```
=> d his

     (FILE 'HOME' ENTERED AT 11:15:44 ON 26 SEP 2006)

     FILE 'REGISTRY' ENTERED AT 11:16:05 ON 26 SEP 2006
L1             STRUCTURE UPLOADED
L2           0 S L1

     FILE 'CAPLUS' ENTERED AT 11:16:51 ON 26 SEP 2006
L3           1 S US20040220164/PN
               SELECT RN L3 1-

     FILE 'REGISTRY' ENTERED AT 11:17:19 ON 26 SEP 2006
L4            41 S E1-41
L5            30 S L4 AND 12/SZ
L6         19728 S 12/SZ
L7            15 S L1  SUB=L6 SAM
L8           221 S L1  SUB=L6 FUL
L9           211 S L8 AND CAPLUS/LC
L10           10 S L8 NOT L9

     FILE 'CAPLUS' ENTERED AT 11:20:21 ON 26 SEP 2006
L11          106 S L8
L12          ANALYZE L11 1- RN HIT :     211 TERMS

     FILE 'REGISTRY' ENTERED AT 11:20:45 ON 26 SEP 2006
L13          100 S 133256?/RN
L14         1088 S 35980?/RN
L15          100 S 182316?/RN
L16          100 S 106415?/RN
L17          100 S 164913?/RN
L18          100 S 182316?/RN
L19          100 S 122114?/RN
L20          100 S 174192?/RN
L21            2 S L8 AND L13
L22            1 S L8 AND L14
L23           16 S L8 AND L15
L24            1 S L8 AND L16
L25            3 S L8 AND L17
L26           16 S L8 AND L18
L27            1 S L8 AND L19
L28            6 S L8 AND L20
L29          217 S L8 NOT (L21 OR L24 OR L27)

     FILE 'CAPLUS' ENTERED AT 11:26:50 ON 26 SEP 2006
L30           83 S L29

=> d l1
L1 HAS NO ANSWERS
L1              STR
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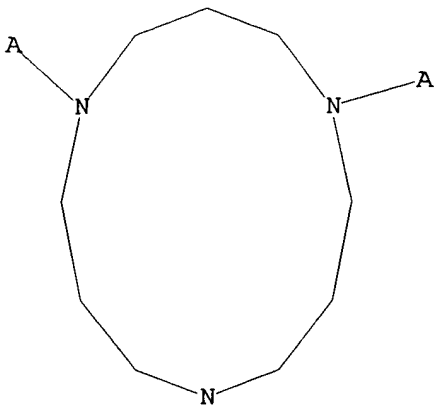
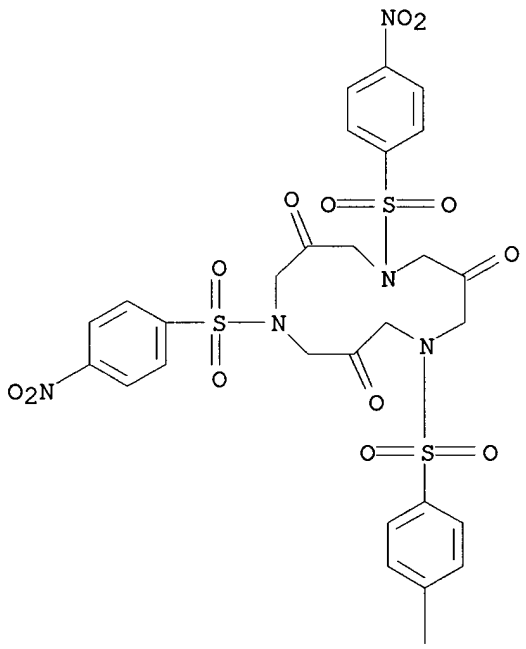


Structure attributes must be viewed using STN Express query preparation.

=> d l10 1-10
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

L10 ANSWER 1 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 907969-73-7 REGISTRY
ED Entered STN: 20 Sep 2006
CN INDEX NAME NOT YET ASSIGNED
MF C27 H24 N6 O15 S3
SR Other Sources
Database: NCI 3D (National Cancer Institute)

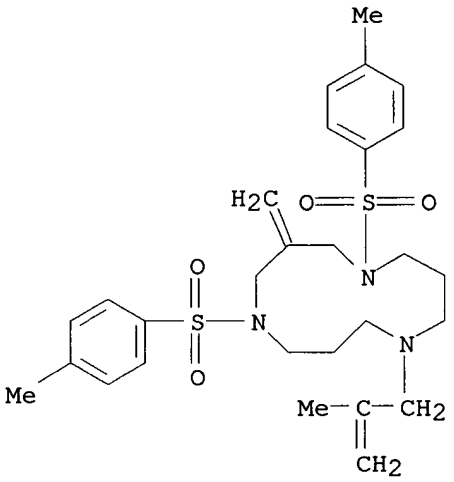
PAGE 1-A



PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

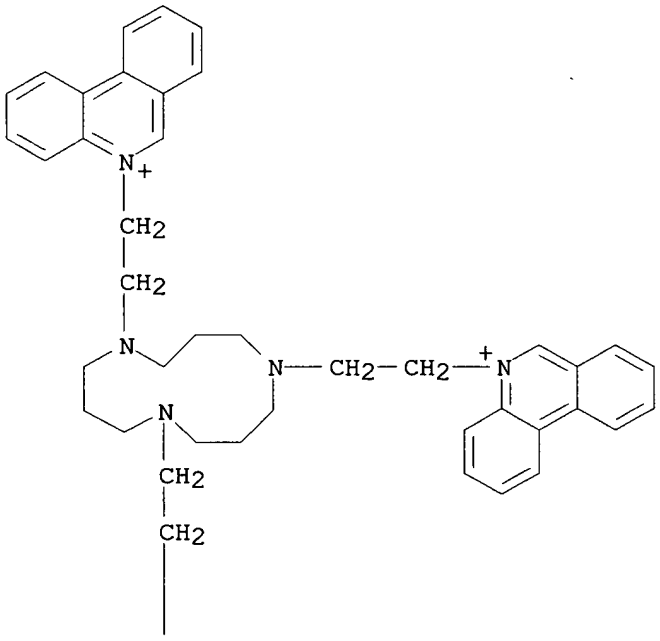
L10 ANSWER 2 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 907960-90-1 REGISTRY
ED Entered STN: 20 Sep 2006
CN INDEX NAME NOT YET ASSIGNED
MF C28 H39 N3 O4 S2
SR Other Sources
Database: NCI 3D (National Cancer Institute)



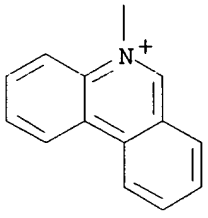
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 ANSWER 3 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 854588-70-8 REGISTRY
ED Entered STN: 12 Jul 2005
CN Phenanthridinium, 5,5',5''-(1,5,9-triazacyclododecane-1,5,9-triyltri-2,1-ethanediyl)tris- (9CI) (CA INDEX NAME)
MF C54 H57 N6
CI COM
SR CA

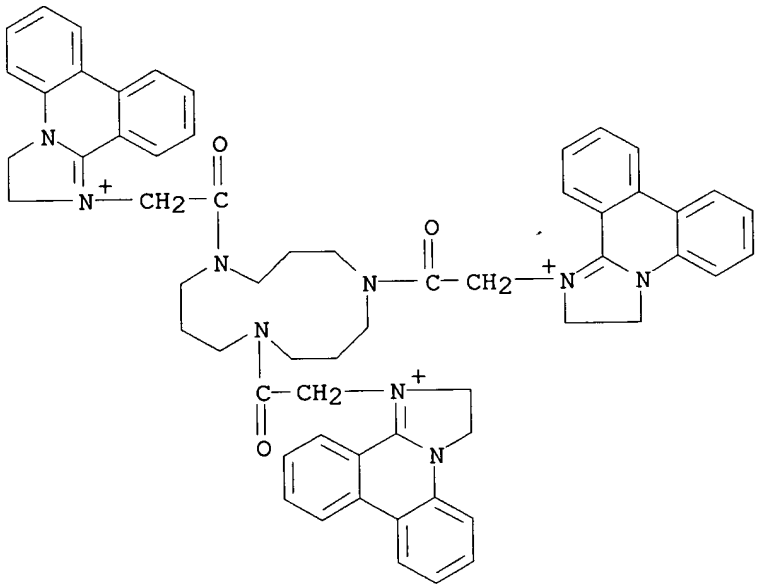
PAGE 1-A



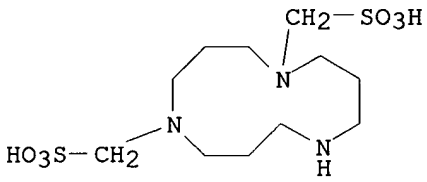
PAGE 2-A



L10 ANSWER 4 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 854588-68-4 REGISTRY
ED Entered STN: 12 Jul 2005
CN Imidazo[1,2-f]phenanthridinium, 1,1',1''-[1,5,9-triazacyclododecane-1,5,9-triyltris(2-oxo-2,1-ethanediyl)]tris[2,3-dihydro- (9CI) (CA INDEX NAME)
MF C60 H60 N9 O3
CI COM
SR CA



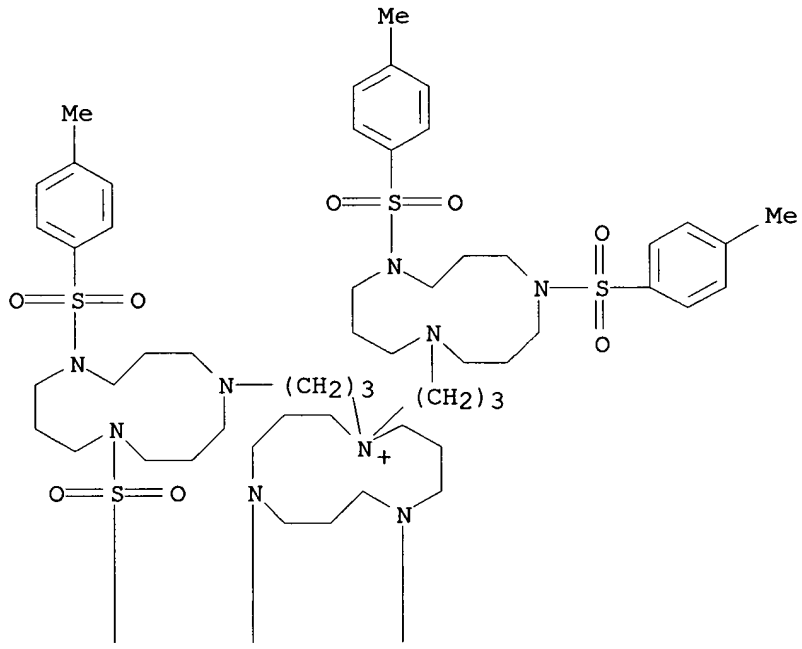
L10 ANSWER 5 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 791560-02-6 REGISTRY
ED Entered STN: 02 Dec 2004
CN 1,5,9-Triazacyclododecane-1,5-dimethanesulfonic acid (9CI) (CA INDEX NAME)
MF C11 H25 N3 O6 S2
CI COM
SR CA



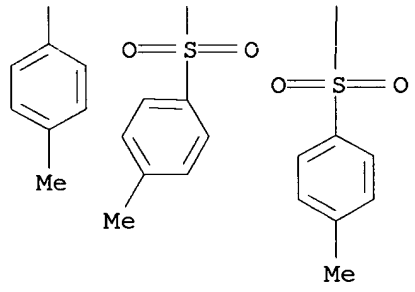
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 ANSWER 6 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 752178-62-4 REGISTRY
ED Entered STN: 26 Sep 2004
CN 5,9-Diaza-1-azoniacyclododecane, 1,1-bis[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)
MF C75 H108 N9 O12 S6
CI COM
SR CA

PAGE 1-A

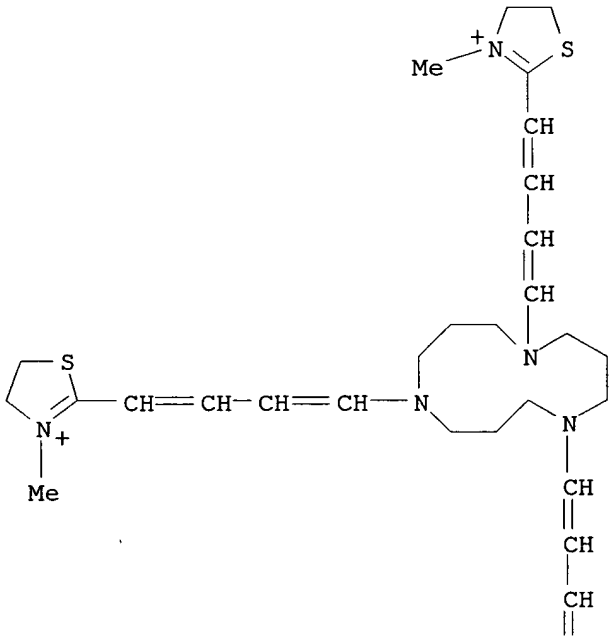


PAGE 2-A

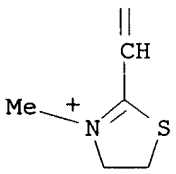


L10 ANSWER 7 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 748118-82-3 REGISTRY
ED Entered STN: 20 Sep 2004
CN Thiazolium, 2,2',2''-(1,5,9-triazacyclododecane-1,5,9-triyltri-1,3-butadiene-4,1-diyl)tris[4,5-dihydro-3-methyl- (9CI) (CA INDEX NAME)
MF C33 H51 N6 S3
CI COM
SR CA

PAGE 1-A

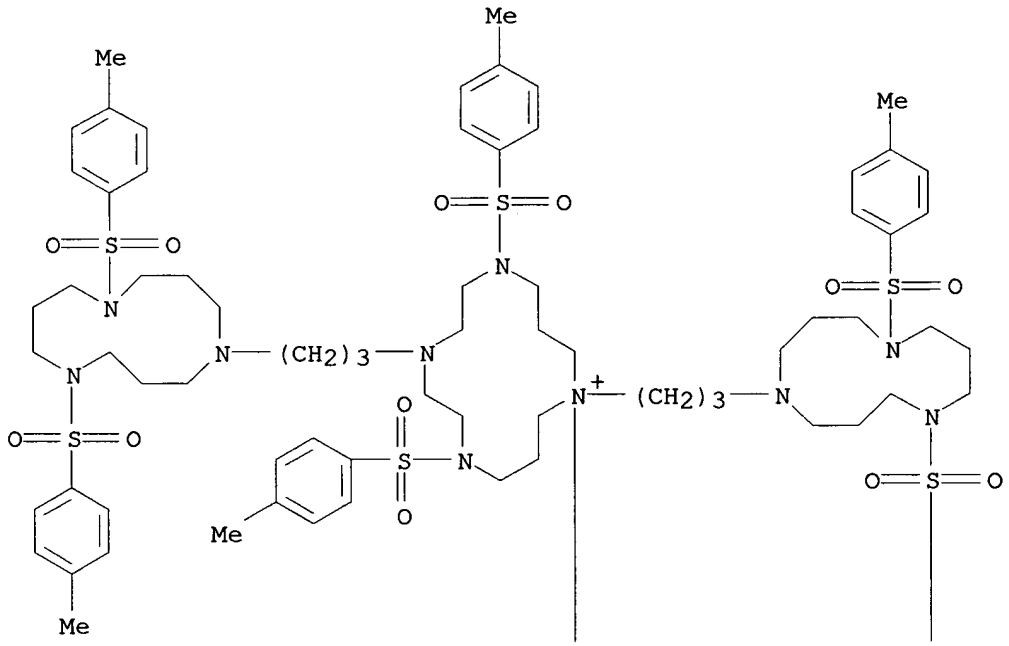


PAGE 2-A

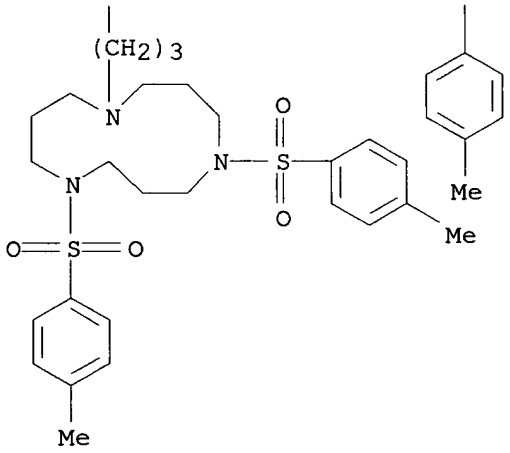


L10 ANSWER 8 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 745771-41-9 REGISTRY
ED Entered STN: 16 Sep 2004
CN 1,4,7-Triaza-11-azoniacyclotetradecane, 4,11,11-tris[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,7-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)
MF C102 H148 N13 O16 S8
CI COM
SR CA

PAGE 1-A

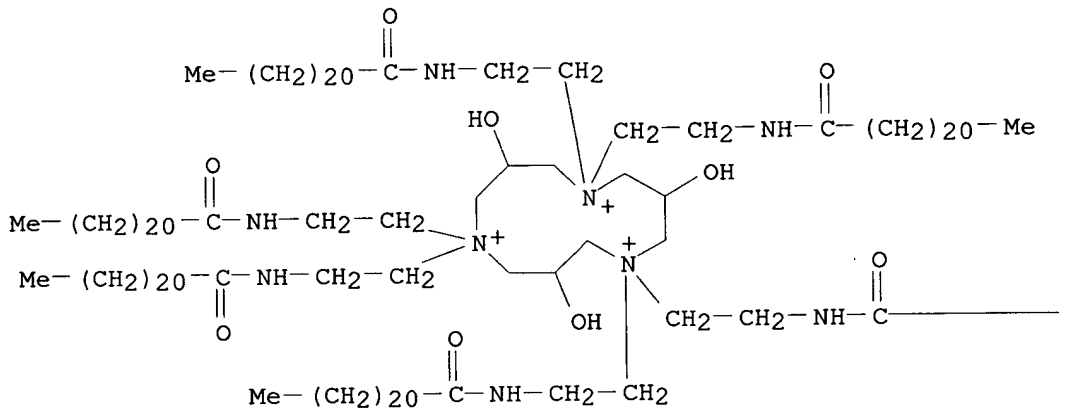


PAGE 2-A



L10 ANSWER 9 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 745760-17-2 REGISTRY
ED Entered STN: 16 Sep 2004
CN 1,5,9-Triazoniacyclododecane, 3,7,11-trihydroxy-1,1,5,5,9,9-hexakis[2-[(1-oxodocosyl)amino]ethyl]-, (9CI) (CA INDEX NAME)
MF C153 H306 N9 O9
CI COM
SR CA

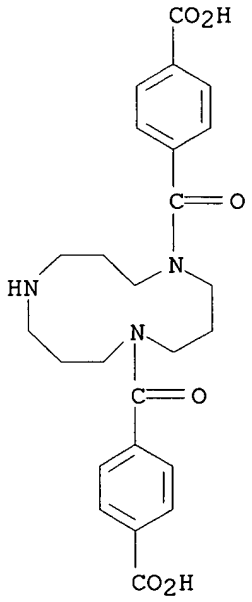
PAGE 1-A



PAGE 1-B

— $(CH_2)_{20}$ — Me

L10 ANSWER 10 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN
RN 132434-01-6 REGISTRY
ED Entered STN: 01 Mar 1991
CN Benzoic acid, 4,4'-(1,5,9-triazacyclododecane-1,5-diyldicarbonyl)bis- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,5,9-Triazacyclododecane, benzoic acid deriv.
MF C25 H29 N3 O6
CI COM
SR CA

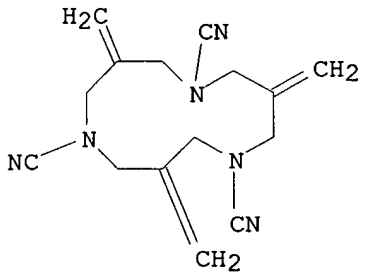


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L80 ANSWER 1 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:357496 CAPLUS
Correction of: 2005:481368
DOCUMENT NUMBER: 145:123918
Correction of: 142:481541
TITLE: Cyanogen halides, cyanates and their sulfur, selenium, and tellurium analogues, sulfinyl and sulfonyl cyanides, cyanamides, and phosphaalkynes
AUTHOR(S): Wu, Y.-Q.
CORPORATE SOURCE: Dept. of Research, Guilford Pharmaceutical, Inc., Baltimore, MD, 21224, USA
SOURCE: Science of Synthesis (2005), 18, 17-63
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review of the preparation of cyanogen halides and cyanates as well as their application to organic synthesis. Sulfur, selenium, and tellurium analogs, sulfinyl and sulfonyl cyanides, cyanamides, and phosphaalkynes are included.

IT 219839-49-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(review preparation and application of cyanogen halides and cyanates as well as numerous derivs. thereof)
RN 219839-49-3 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarbonitrile, 3,7,11-tris(methylene)- (9CI) (CA INDEX NAME)

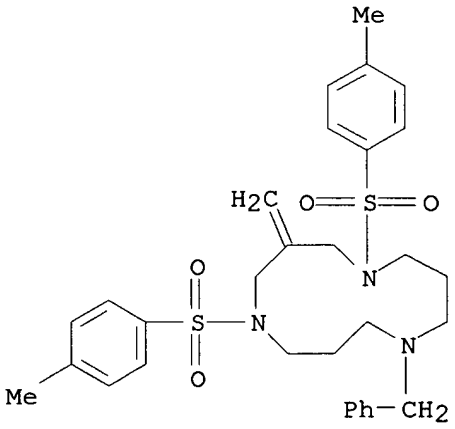


L30 ANSWER 2 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:240977 CAPLUS
DOCUMENT NUMBER: 144:246374
TITLE: Inhibitors of HIV infection via the cellular CD4 receptor
AUTHOR(S): Vermeire, Kurt; Schols, Dominique; Bell, Thomas W.
CORPORATE SOURCE: Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.
SOURCE: Current Medicinal Chemistry (2006), 13(7), 731-743
CODEN: CMCHE7; ISSN: 0929-8673
PUBLISHER: Bentham Science Publishers Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review. Recent advances in the understanding of cellular and mol. mechanisms of viral penetration of the target cell have provided the basis for novel chemotherapy and prophylaxis of HIV-1 infections. This knowledge has been successfully applied to the development of inhibitors that target discrete steps of the entry process. Interesting approaches for the prevention of HIV-1 entry include the use of small-mol. inhibitors, natural ligands, and(or) monoclonal antibodies that interfere with gp120/CD4 interaction. Other compds. acting by novel mechanisms have recently been identified as anti-HIV agents and seem worthy of further preclin. development. Of particular interest in this regard are cyclotriazadisulfonamide (CADA) compds., which down-modulate the cellular receptor, CD4. A series of analogs of 9-benzyl-3-methylene-1,5-di-p-toluenesulfonyl-1,5,9-triazacyclododecane (CADA) has been synthesized and tested for CD4 down-modulation and anti-HIV activity. Some derivs. proved to be highly effective in decreasing cellular CD4 and in acting as HIV entry inhibitors. Three-dimensional quant. structure-activity relationship (3D-QSAR) studies correlating mol. features with potency have been used to produce a computational model. This model can be used to design more potent CD4 down-modulating drugs for HIV therapy and prophylaxis. This review summarizes the results of recent studies relating to inhibitors of HIV infection via CD4 and discusses the therapeutic potential of targeting this cellular receptor. Special attention is given to the aothors' own work on small-mol. HIV entry inhibitors endowed with CD4 down-modulating properties.

IT 182316-44-5, CADA
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibitors of HIV infection via cellular CD4 receptor)

RN 182316-44-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



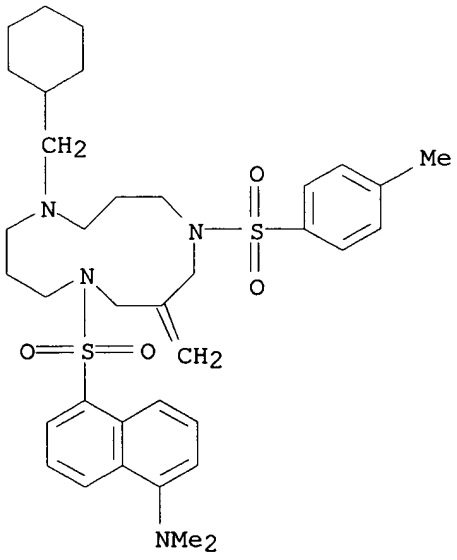
REFERENCE COUNT: 102 THERE ARE 102 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 3 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:94623 CAPLUS
DOCUMENT NUMBER: 144:350657
TITLE: Synthesis and Structure-Activity Relationship Studies of CD4 Down-Modulating Cyclotriazadisulfonamide (CADA) Analogues
AUTHOR(S): Bell, Thomas W.; Anugu, Sreenivasa; Bailey, Patrick; Catalano, Vincent J.; Dey, Kaka; Drew, Michael G. B.; Duffy, Noah H.; Jin, Qi; Samala, Meinrado F.; Sodoma, Andrej; Welch, William H.; Schols, Dominique; Vermeire, Kurt
CORPORATE SOURCE: Departments of Chemistry and Biochemistry, University of Nevada, Reno, NV, 89557, USA
SOURCE: Journal of Medicinal Chemistry (2006), 49(4), 1291-1312
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:350657

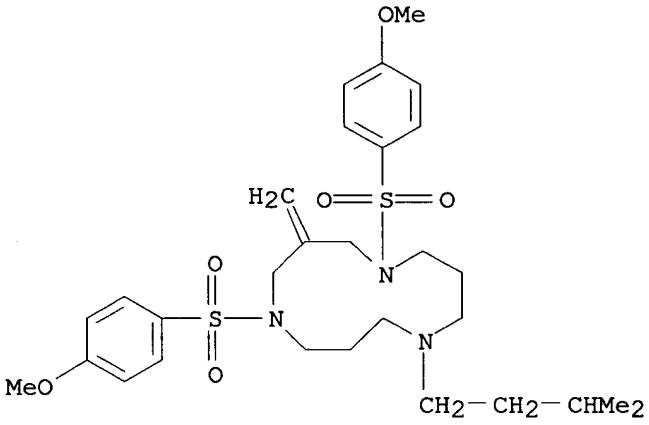
AB HIV attachment via the CD4 receptor is an important target for developing novel approaches to HIV chemotherapy. Cyclotriazadisulfonamide (CADA) inhibits HIV at sub-micromolar levels by specifically down-modulating cell-surface and intracellular CD4. An effective five-step synthesis of CADA in 30% overall yield is reported. This synthesis has also been modified to produce more than 50 analogs. Many tail-group analogs have been made by removing the benzyl tail of CADA and replacing it with various alkyl, acyl, alkoxycarbonyl and aminocarbonyl substituents. A series of sidearm analogs, including two unsym. compds., have also been prepared by modifying the CADA synthesis, replacing the toluenesulfonyl sidearms with other sulfonyl groups. Testing 30 of these compds. in MT-4 cells shows a wide range of CD4 down-modulation potency, which correlates with ability to inhibit HIV-1. Three-dimensional quant. structure-activity relationship (3D-QSAR) models were constructed using comparative mol. field anal. (CoMFA) and comparative mol. similarity indexes anal. (CoMSIA) approaches. The X-ray crystal structures of four compds., including CADA, show the same major conformation of the central 12-membered ring. The solid-state structure of CADA was energy minimized and used to generate the remaining 29 structures, which were similarly minimized and aligned to produce the 3D-QSAR models. Both models indicate that steric bulk of the tail group, and, to a lesser extent, the sidearms mainly determine CD4 down-modulation potency in this series of compds.

IT 471866-80-5P 881693-80-7P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and structure-activity relationship study of CD4 down-modulating cyclotriazadisulfonamide (CADA) analogs)

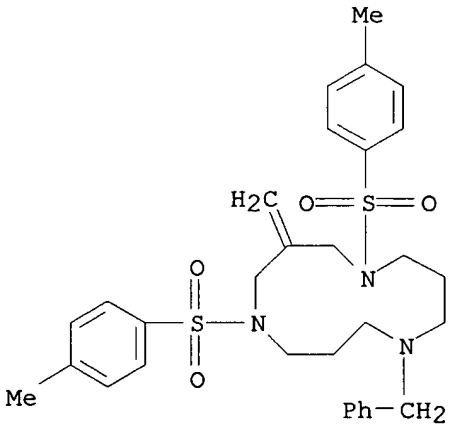
RN 471866-80-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(cyclohexylmethyl)-1-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]-3-methylene-5-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



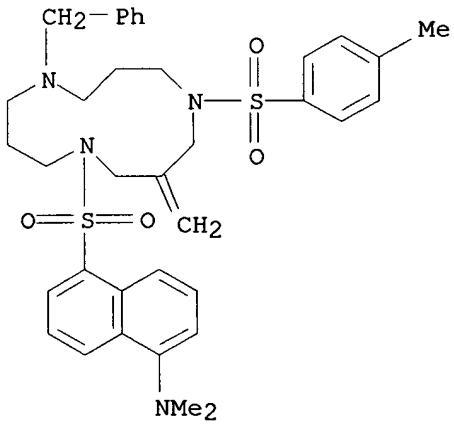
RN 881693-80-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methoxyphenyl)sulfonyl]-9-(3-methylbutyl)-3-methylene- (9CI) (CA INDEX NAME)



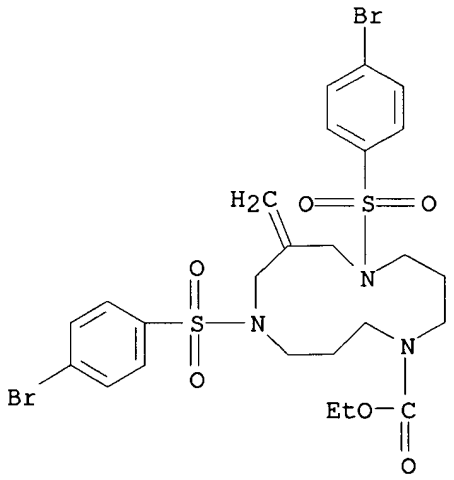
IT 182316-44-5DP, CADA, analogs 471866-79-2P
881693-78-3P 881693-79-4P 881693-81-8P
881693-82-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and structure-activity relationship study of CD4 down-modulating cyclotriazadisulfonamide (CADA) analogs)
RN 182316-44-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



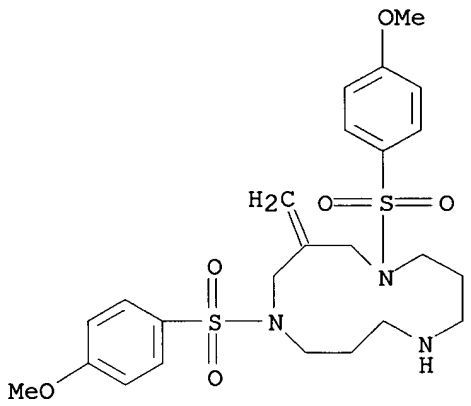
RN 471866-79-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 1-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]-3-methylene-5-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



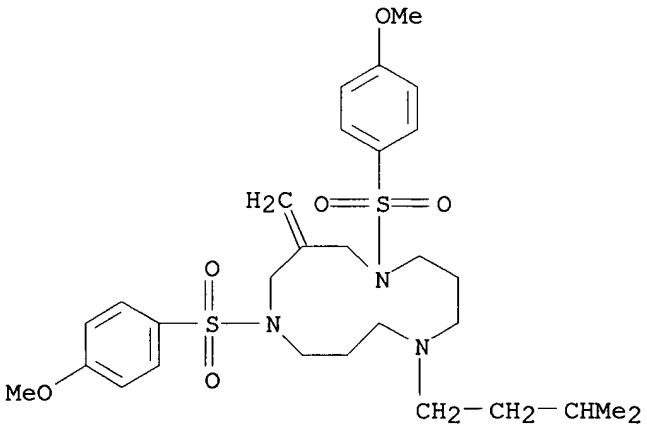
RN 881693-78-3 CAPLUS
CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 5,9-bis[(4-bromophenyl)sulfonyl]-7-methylene-, ethyl ester (9CI) (CA INDEX NAME)



RN 881693-79-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methoxyphenyl)sulfonyl]-3-methylene- (9CI) (CA INDEX NAME)

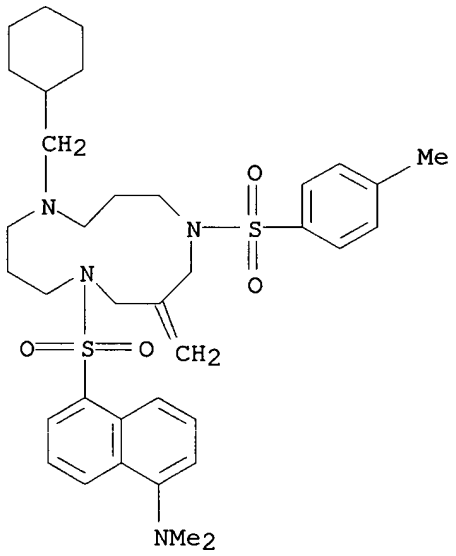


RN 881693-81-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methoxyphenyl)sulfonyl]-9-(3-methylbutyl)-3-methylene-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 881693-82-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(cyclohexylmethyl)-1-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]-3-methylene-5-[(4-methylphenyl)sulfonyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

IT 182316-34-3P 182316-50-3P 392287-04-6P
471866-90-7P 471866-91-8P 471866-93-0P
471866-97-4P 471867-00-2P 471867-03-5P
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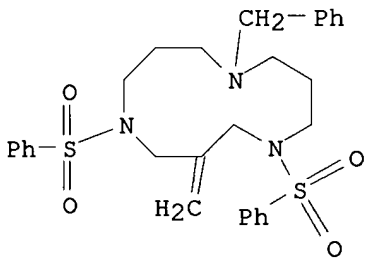
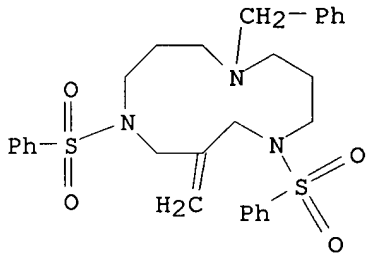
881693-58-9P 881693-59-0P 881693-62-5P
881693-72-7P 881693-74-9P 881693-76-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and structure-activity relationship study of CD4 down-modulating cyclotriazadisulfonamide (CADA) analogs)

RN 182316-34-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-9-(phenylmethyl)-1,5-bis(phenylsulfonyl)- (9CI) (CA INDEX NAME)

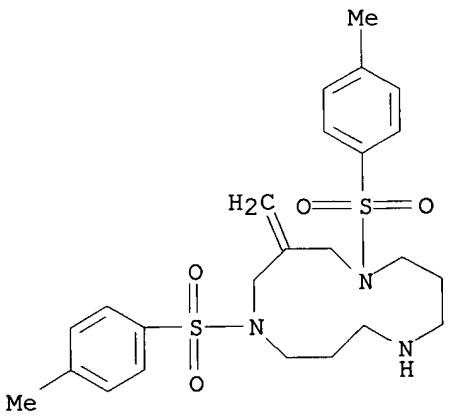


RN 182316-50-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-9-(phenylmethyl)-1,5-bis(phenylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)



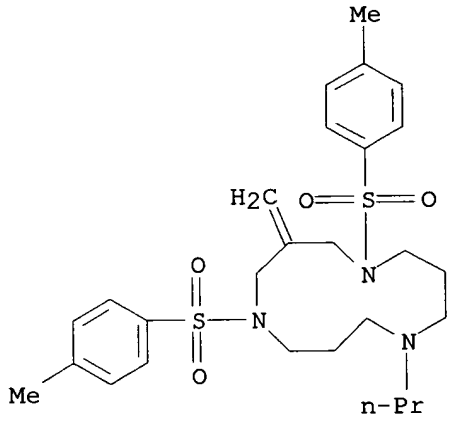
● HCl

RN 392287-04-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

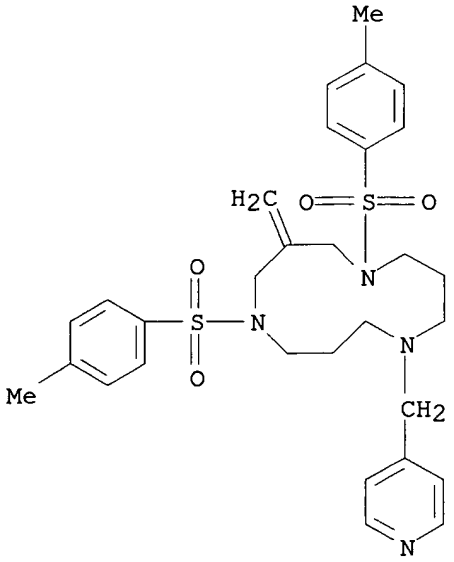


● HCl

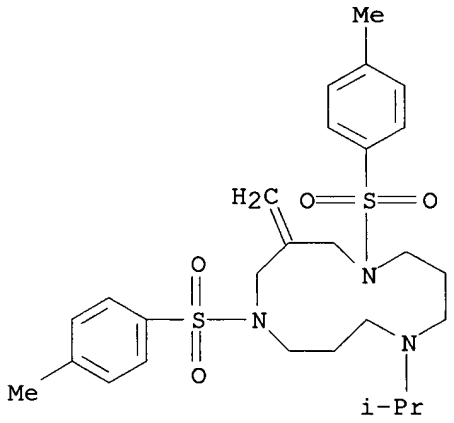
RN 471866-90-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-propyl- (9CI) (CA INDEX NAME)



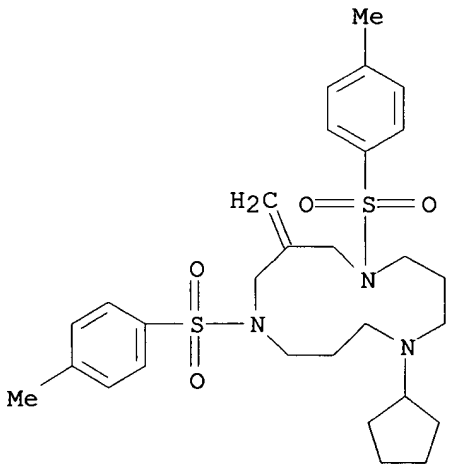
RN 471866-91-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



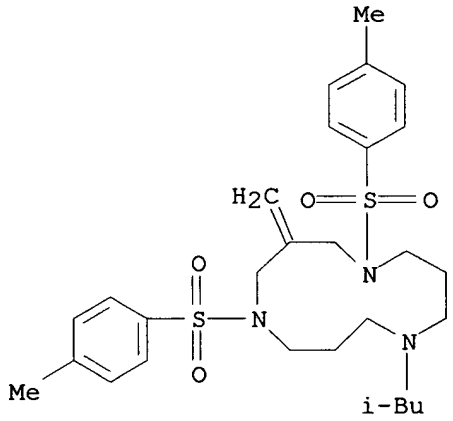
RN 471866-93-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-9-(1-methylethyl)-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



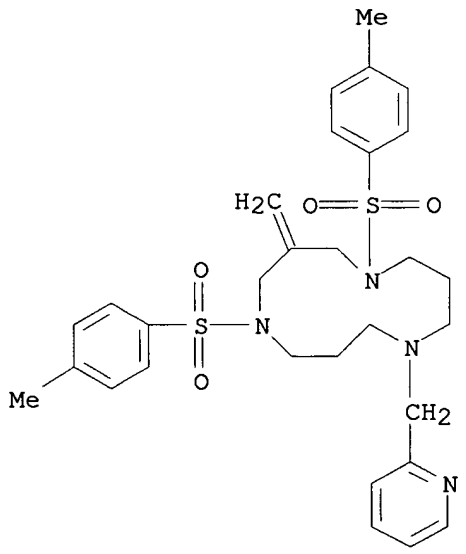
RN 471866-97-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-cyclopentyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



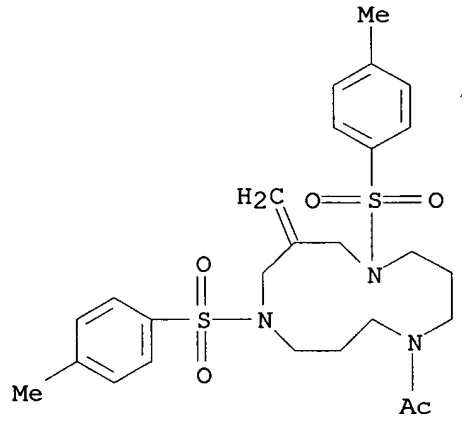
RN 471867-00-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-methylpropyl)- (9CI) (CA INDEX NAME)



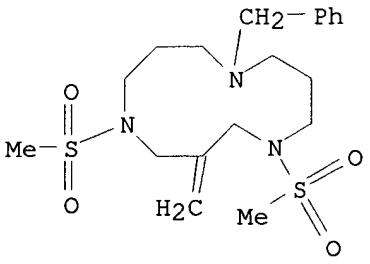
RN 471867-03-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



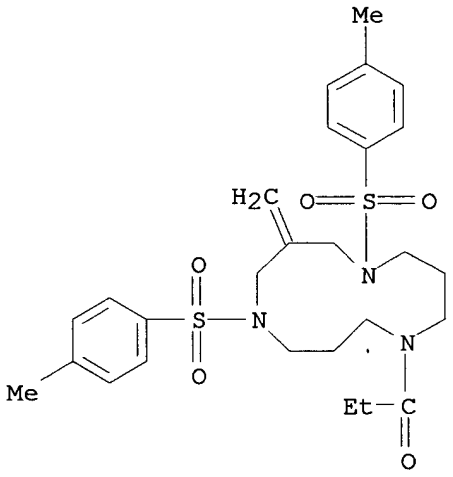
RN 471867-04-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-acetyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



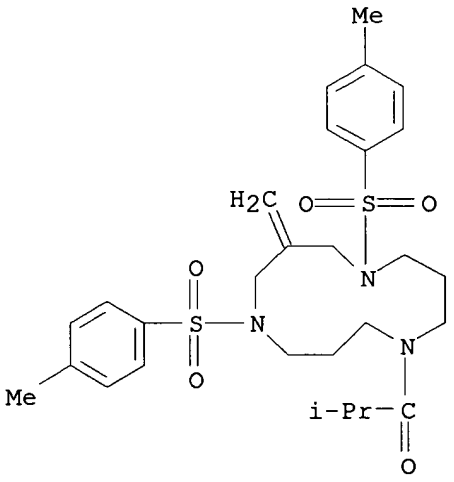
RN 471867-06-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis(methylsulfonyl)-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



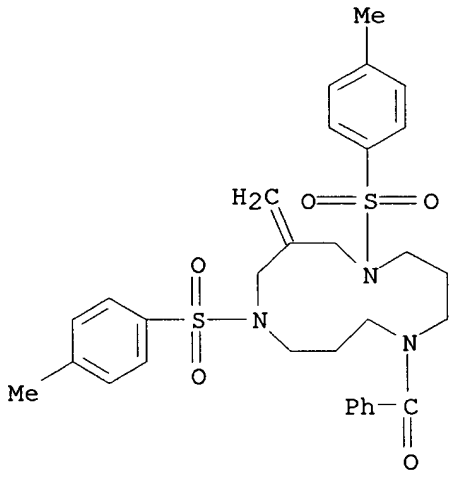
RN 881693-37-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(1-oxopropyl)- (9CI) (CA INDEX NAME)



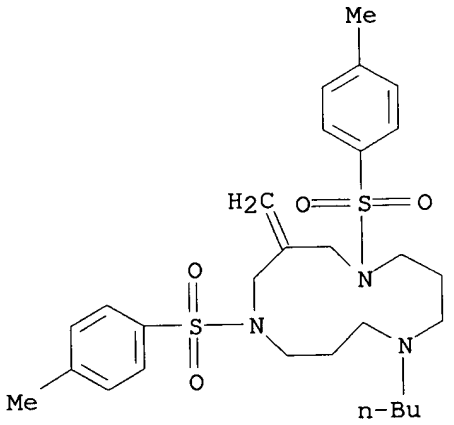
RN 881693-38-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-9-(2-methyl-1-oxopropyl)-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 881693-39-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-benzoyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

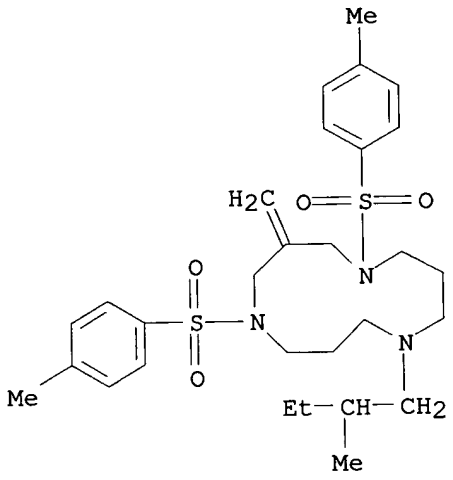


RN 881693-54-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-butyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



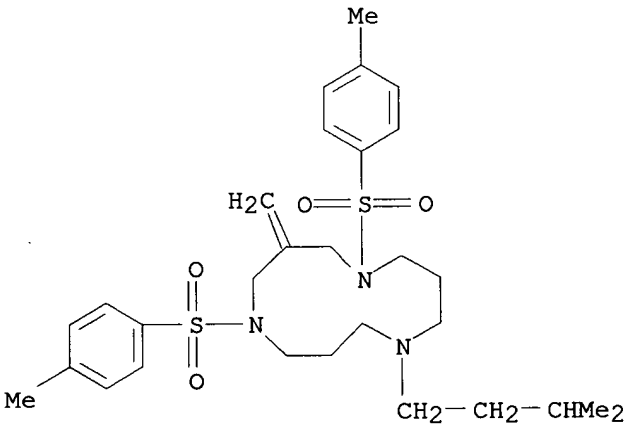
● HCl

RN 881693-55-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(2-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



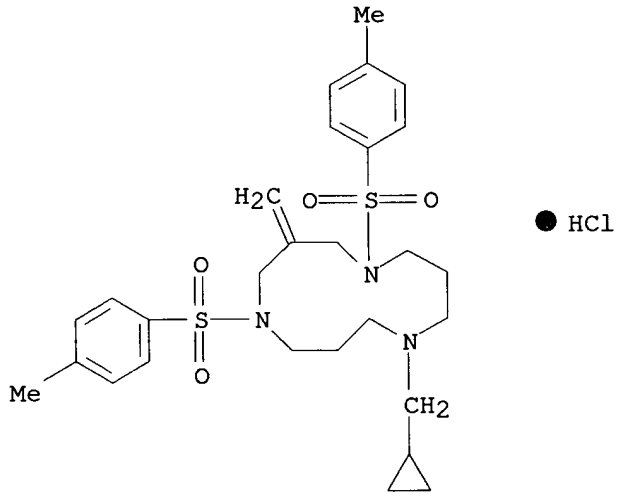
● HCl

RN 881693-56-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(3-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



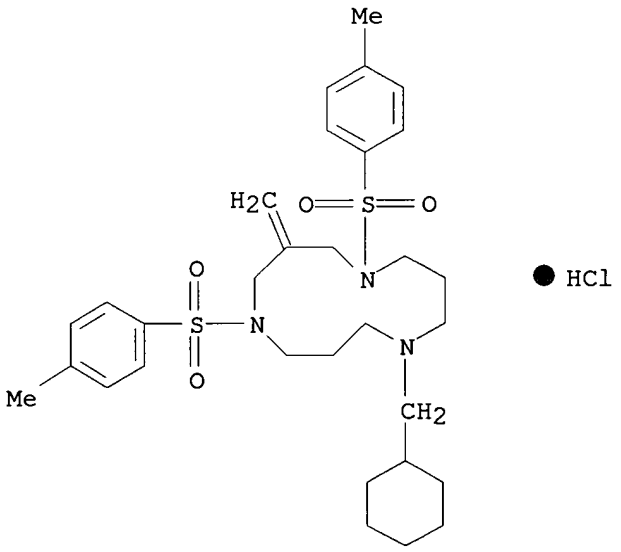
● HCl

RN 881693-57-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(cyclopropylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

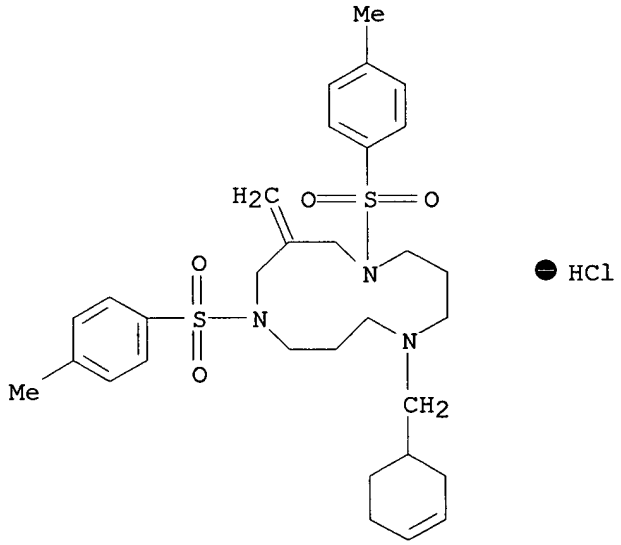


● HCl

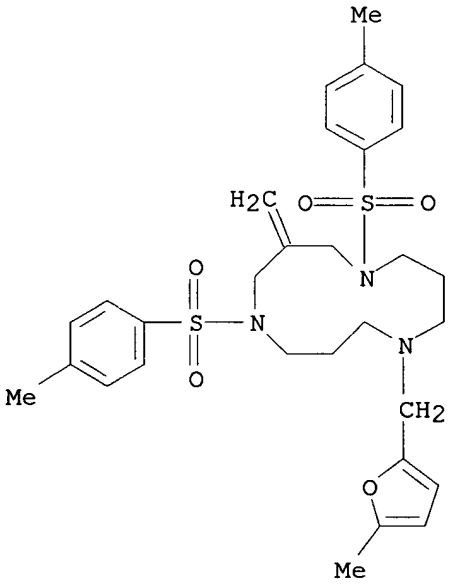
RN 881693-58-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(cyclohexylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



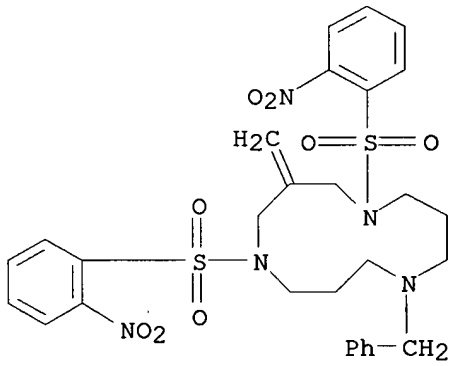
RN 881693-59-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(3-cyclohexen-1-ylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



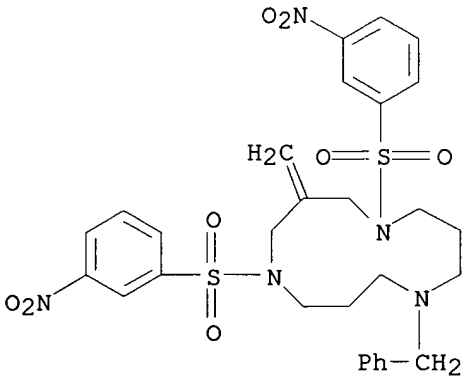
RN 881693-62-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-9-[(5-methyl-2-furanyl)methyl]-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



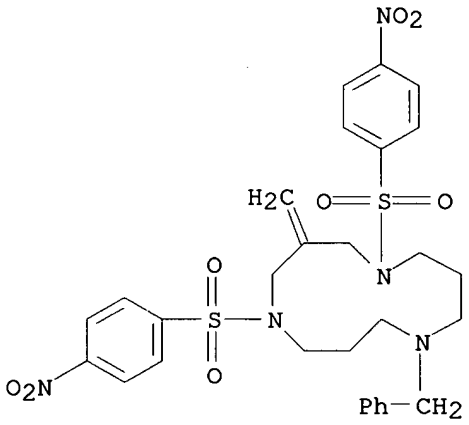
RN 881693-72-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(2-nitrophenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



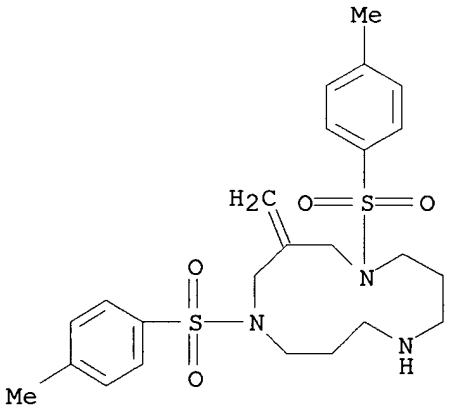
RN 881693-74-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(3-nitrophenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



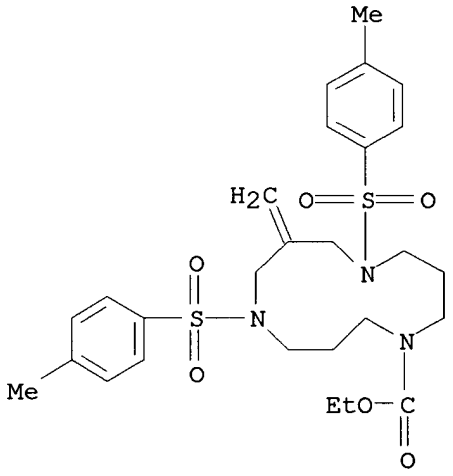
RN 881693-76-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-nitrophenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



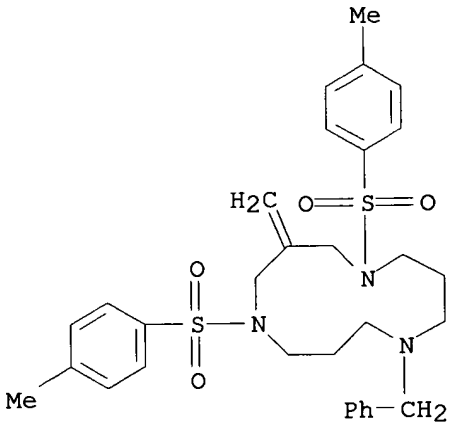
IT 182316-06-9P 182316-30-9P 392287-03-5P
471866-86-1P 471866-87-2P 471866-89-4P
471866-92-9P 471866-94-1P 471866-95-2P
471866-96-3P 471866-98-5P 471867-05-7P
881693-25-0P 881693-26-1P 881693-27-2P
881693-28-3P 881693-29-4P 881693-30-7P
881693-31-8P 881693-32-9P 881693-33-0P
881693-34-1P 881693-36-3P 881693-40-9P
881693-41-0P 881693-42-1P 881693-50-1P
881693-51-2P 881693-52-3P 881693-53-4P
881693-60-3P 881693-61-4P 881693-63-6P
881693-64-7P 881693-65-8P 881693-66-9P
881693-70-5P 881693-73-8P 881693-75-0P
881693-77-2P 881693-83-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and structure-activity relationship study of CD4 down-modulating cyclotriazadisulfonamide (CADA) analogs)
RN 182316-06-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-(9CI) (CA INDEX NAME)



RN 182316-30-9 CAPLUS
CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)

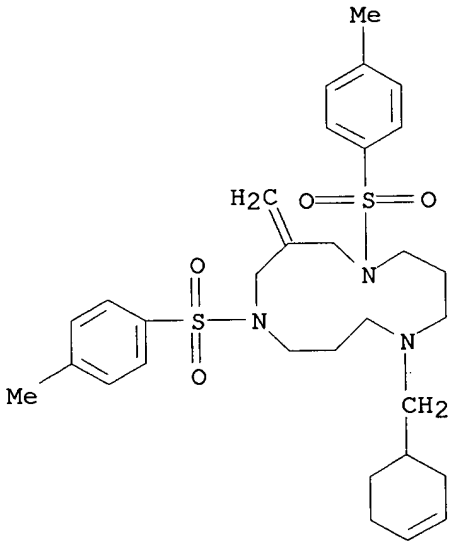


RN 392287-03-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

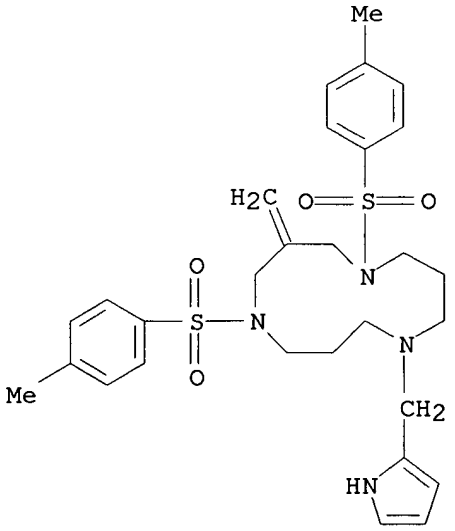


● HCl

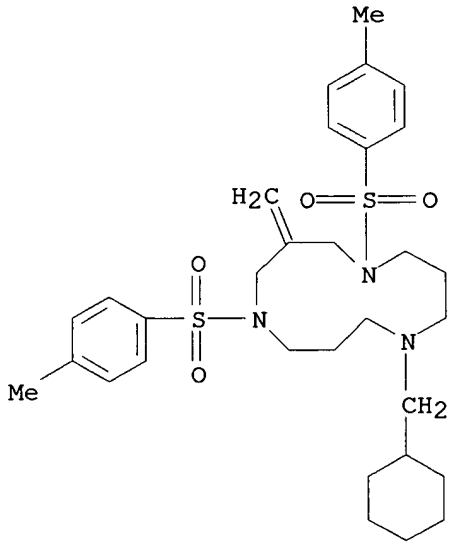
RN 471866-86-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(3-cyclohexen-1-ylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



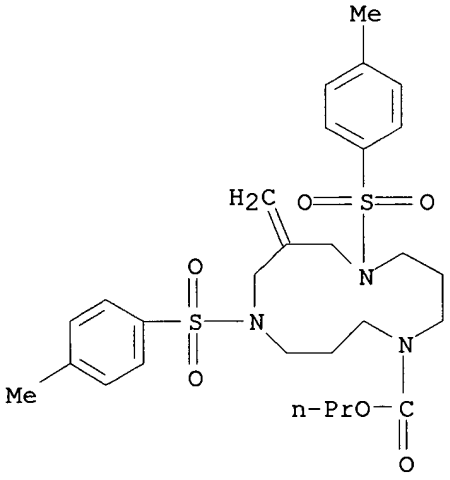
RN 471866-87-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(1H-pyrrol-2-ylmethyl)- (9CI) (CA INDEX NAME)



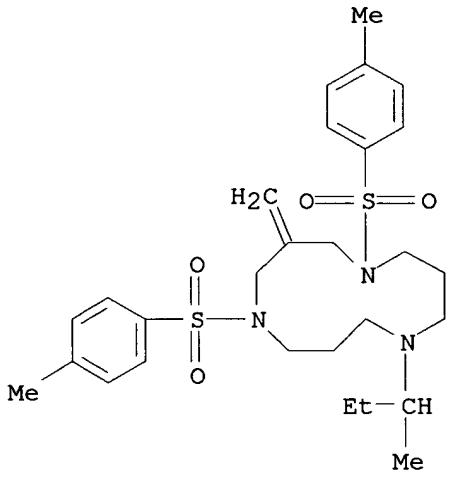
RN 471866-89-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(cyclohexylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



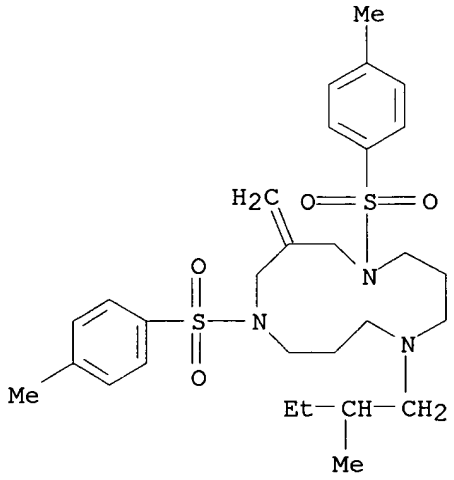
RN 471866-92-9 CAPLUS
CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, propyl ester (9CI) (CA INDEX NAME)



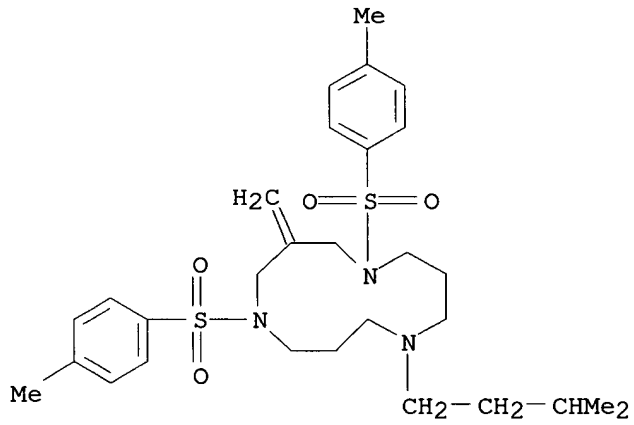
RN 471866-94-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(1-methylpropyl)- (9CI) (CA INDEX NAME)



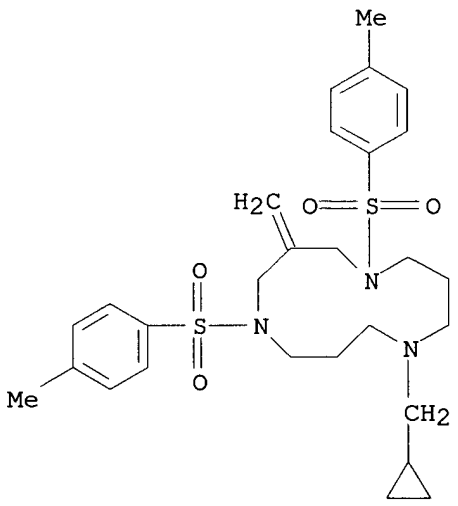
RN 471866-95-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(2-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



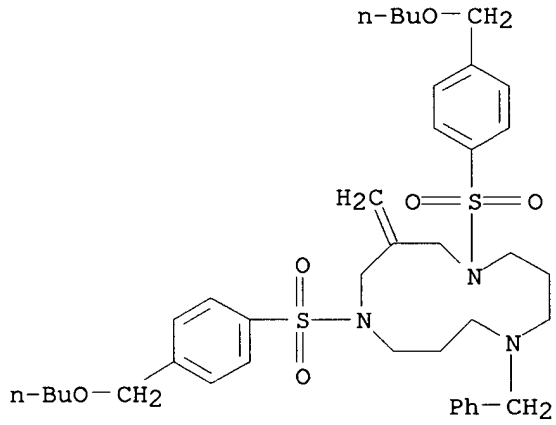
RN 471866-96-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(3-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



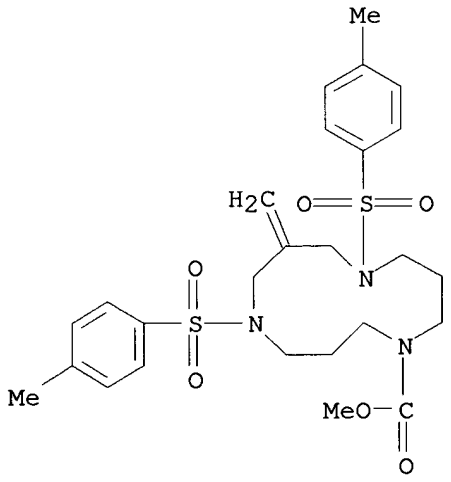
RN 471866-98-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(cyclopropylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



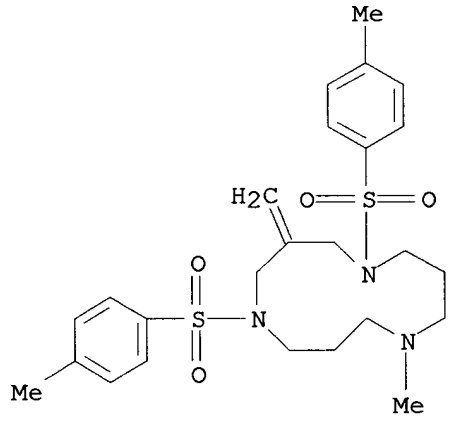
RN 471867-05-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[[4-(butoxymethyl)phenyl]sulfonyl]-3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



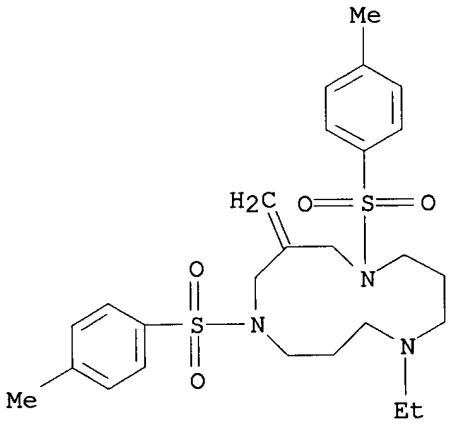
RN 881693-25-0 CAPLUS
CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)



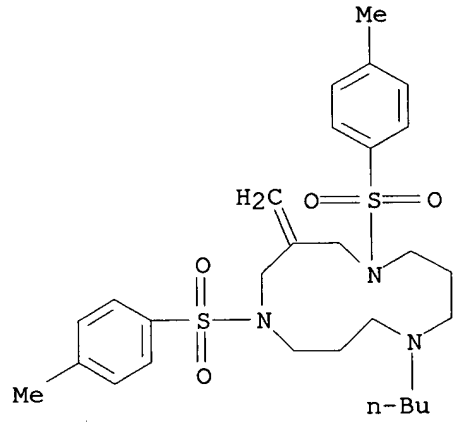
RN 881693-26-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-methyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



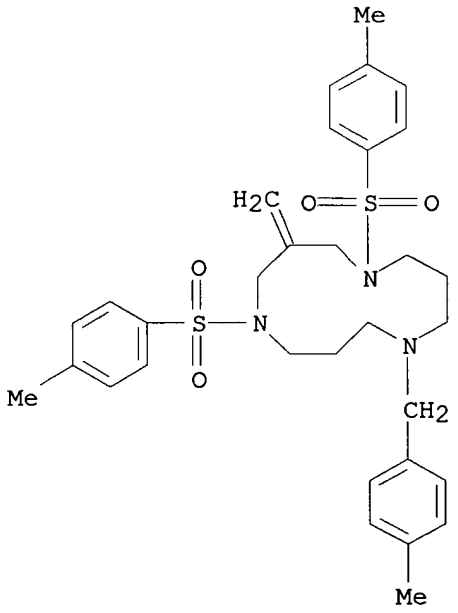
RN 881693-27-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-ethyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



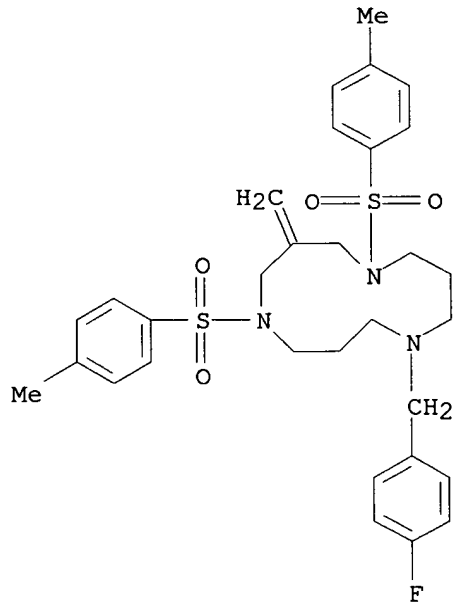
RN 881693-28-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-butyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



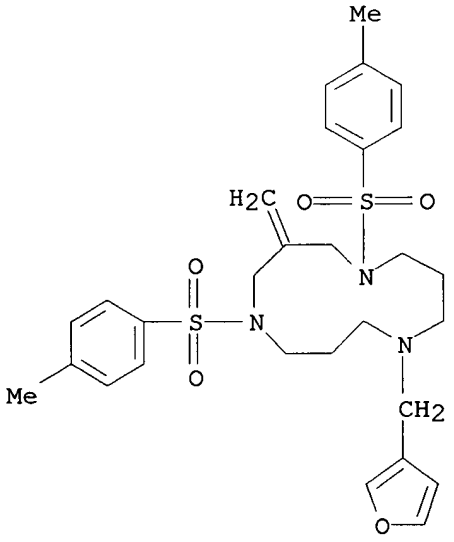
RN 881693-29-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-9-[(4-methylphenyl)methyl]-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



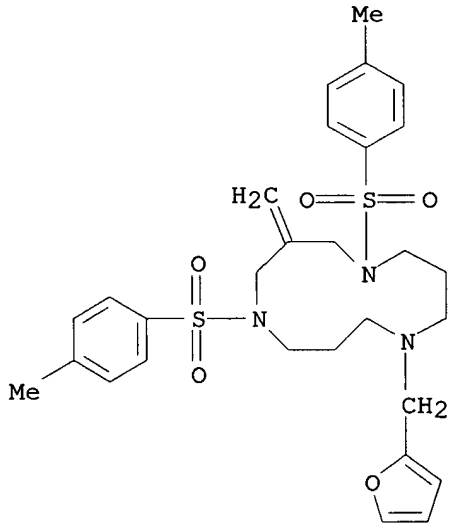
RN 881693-30-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-[(4-fluorophenyl)methyl]-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



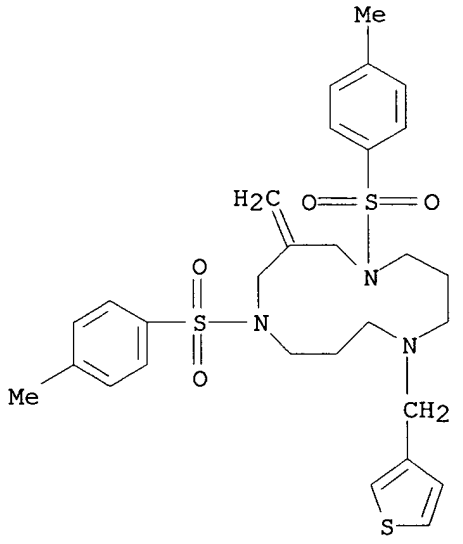
RN 881693-31-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(3-furanylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



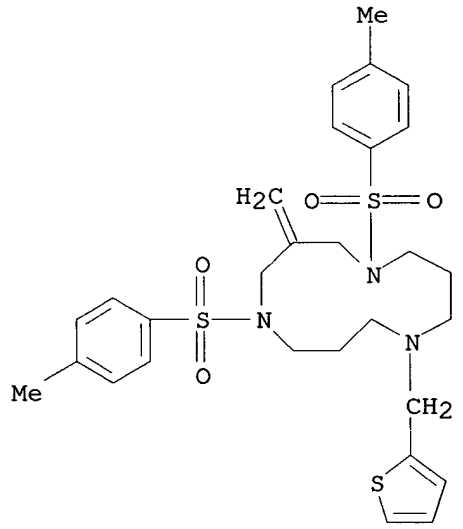
RN 881693-32-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(2-furanylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



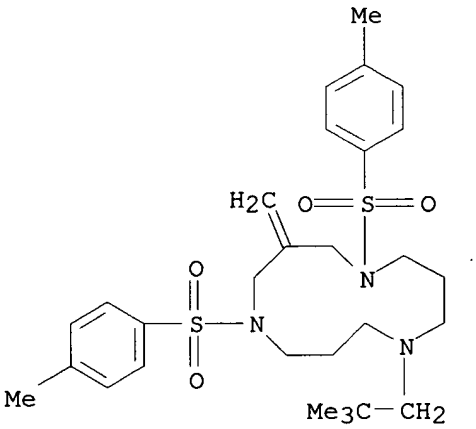
RN 881693-33-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(3-thienylmethyl)- (9CI) (CA INDEX NAME)



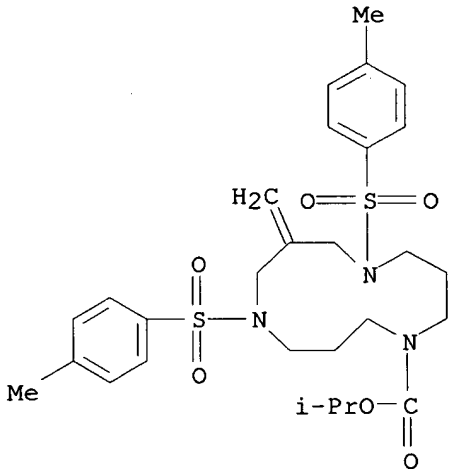
RN 881693-34-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-thienylmethyl)- (9CI) (CA INDEX NAME)



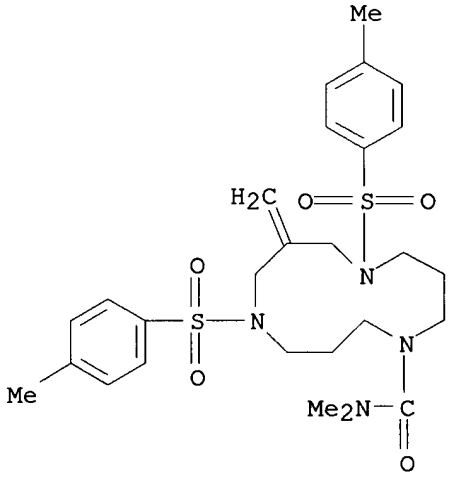
RN 881693-36-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(2,2-dimethylpropyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



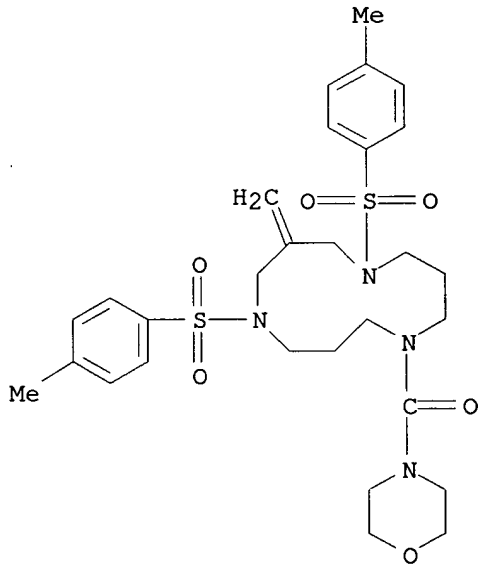
RN 881693-40-9 CAPLUS
CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)



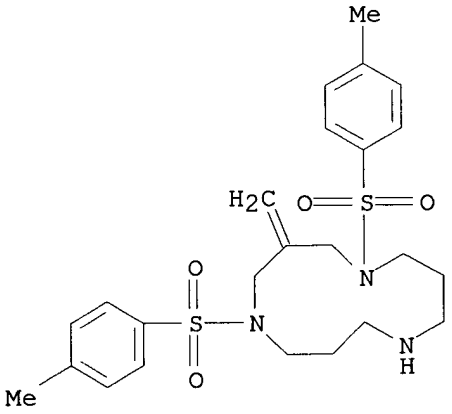
RN 881693-41-0 CAPLUS
CN 1,5,9-Triazacyclododecane-1-carboxamide, N,N-dimethyl-7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 881693-42-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(4-morpholinylcarbonyl)- (9CI) (CA INDEX NAME)

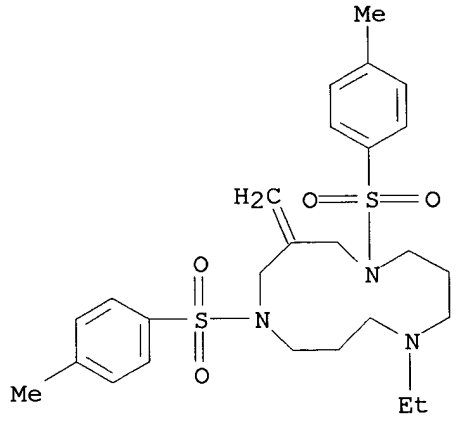


RN 881693-50-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, dihydrochloride (9CI) (CA INDEX NAME)



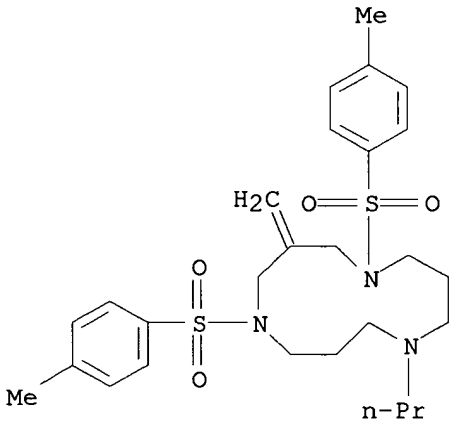
● 2 HCl

RN 881693-51-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-ethyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



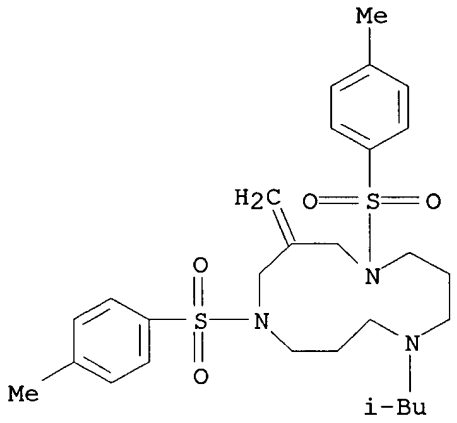
● HCl

RN 881693-52-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-propyl-, monohydrochloride (9CI) (CA INDEX NAME)



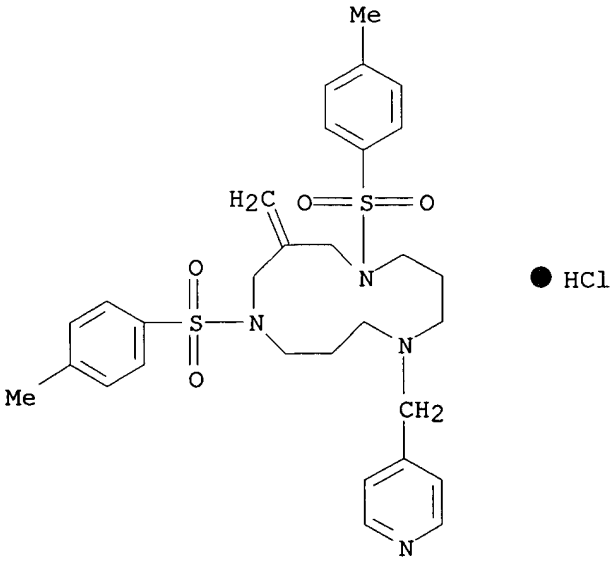
● HCl

RN 881693-53-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-methylpropyl)-, monohydrochloride (9CI) (CA INDEX NAME)

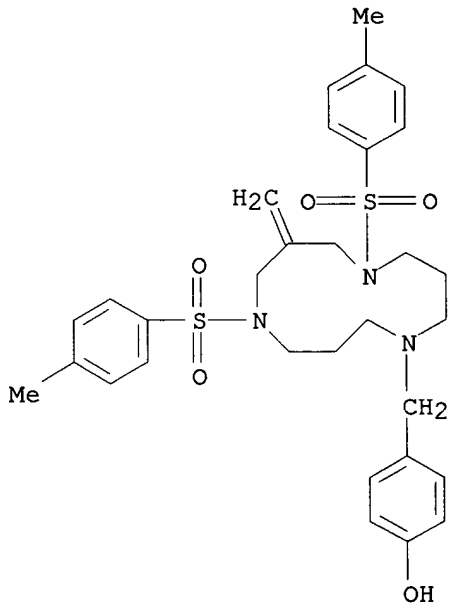


● HCl

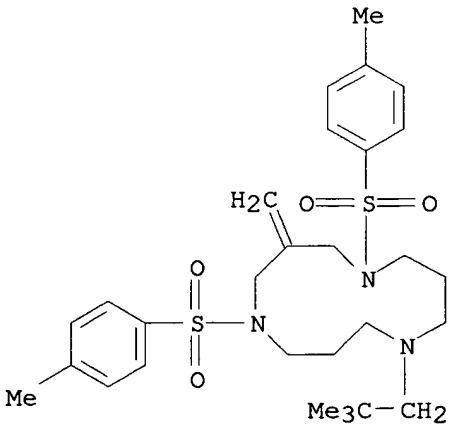
RN 881693-60-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(4-pyridinylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



RN 881693-61-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-[(4-hydroxyphenyl)methyl]-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

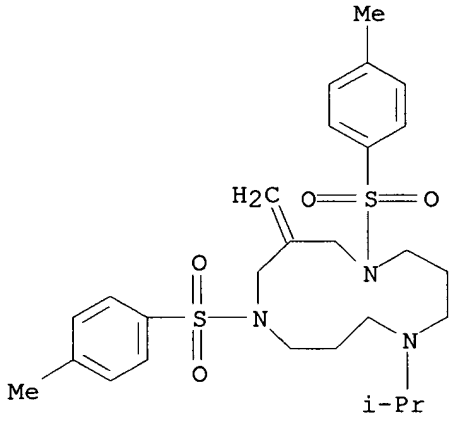


RN 881693-63-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(2,2-dimethylpropyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



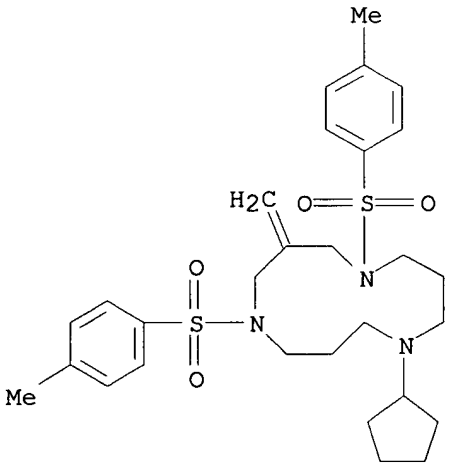
● HCl

RN 881693-64-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-9-(1-methylethyl)-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



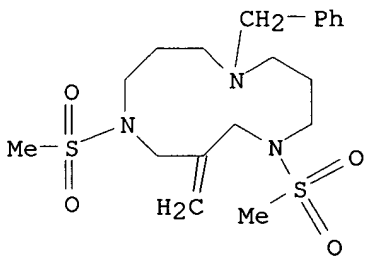
● HCl

RN 881693-65-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-cyclopentyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



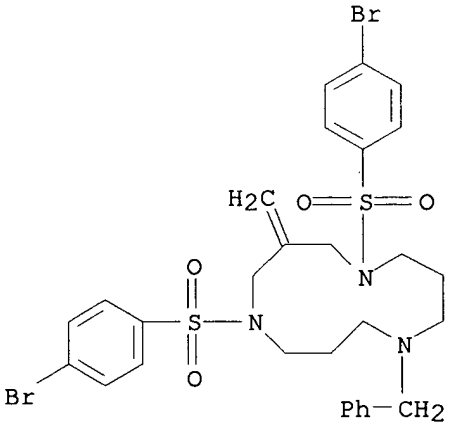
● HCl

RN 881693-66-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis(methylsulfonyl)-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



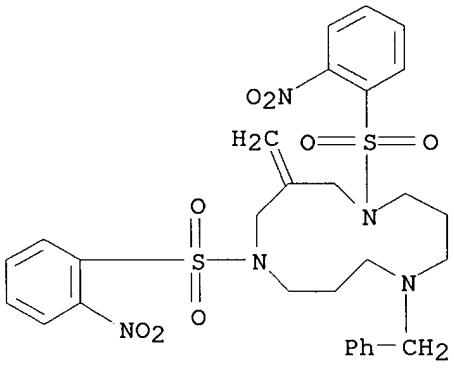
● HCl

RN 881693-70-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-bromophenyl)sulfonyl]-3-methylene-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



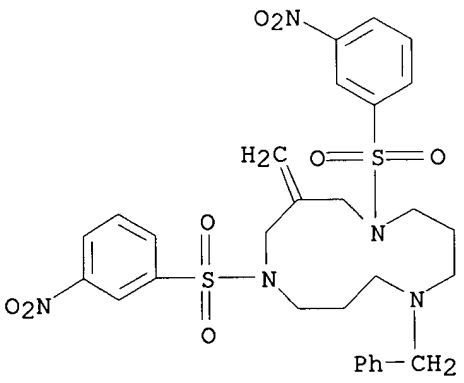
● HCl

RN 881693-73-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(2-nitrophenyl)sulfonyl]-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



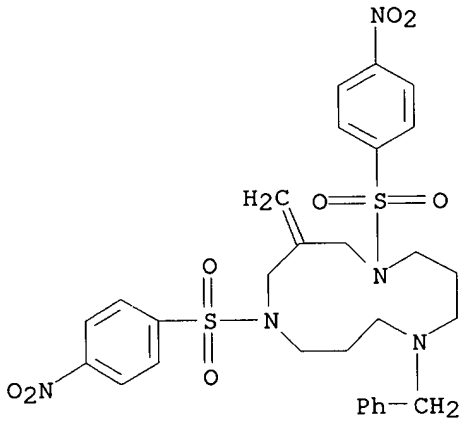
● HCl

RN 881693-75-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(3-nitrophenyl)sulfonyl]-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



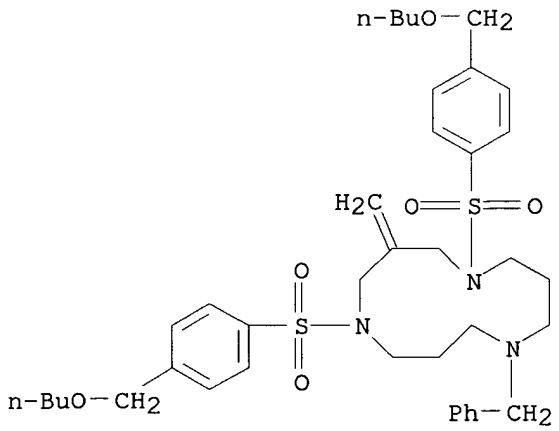
● HCl

RN 881693-77-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-nitrophenyl)sulfonyl]-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



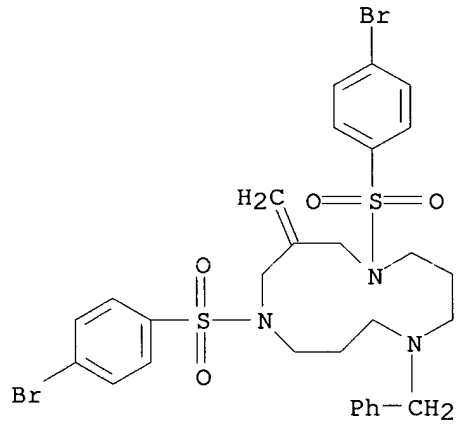
● HCl

RN 881693-83-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[[4-(butoxymethyl)phenyl]sulfonyl]-3-methylene-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



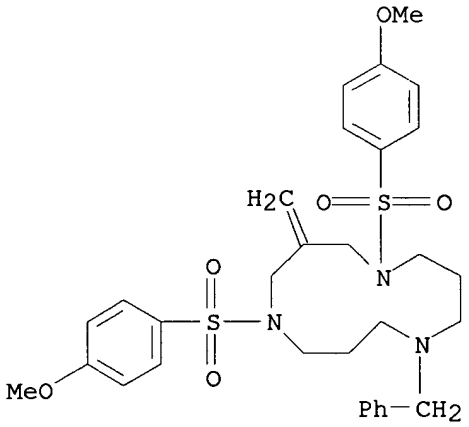
● HCl

IT 471867-02-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (methylene)bis[(bromophenyl)sulfonyl]-1,5,9-triazacyclododecane (ASPB-127) and study of its crystal and mol. structures)
RN 471867-02-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-bromophenyl)sulfonyl]-3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

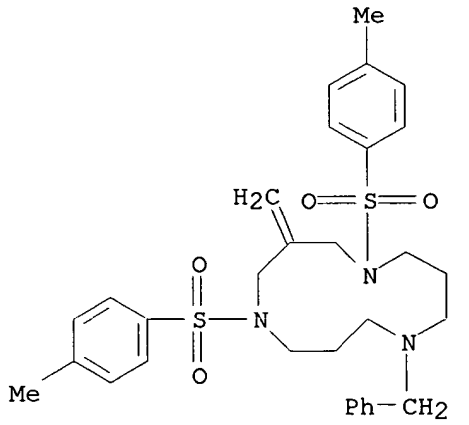


IT 881693-71-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of (methylene)bis[(bromophenyl)sulfonyl]-1,5,9-triazacyclododecane (KKD-023), study of its crystal and mol. structures and its CD4 down-modulating structure-activity relationship study with CADA analogs)
RN 881693-71-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methoxyphenyl)sulfonyl]-3-methylene-

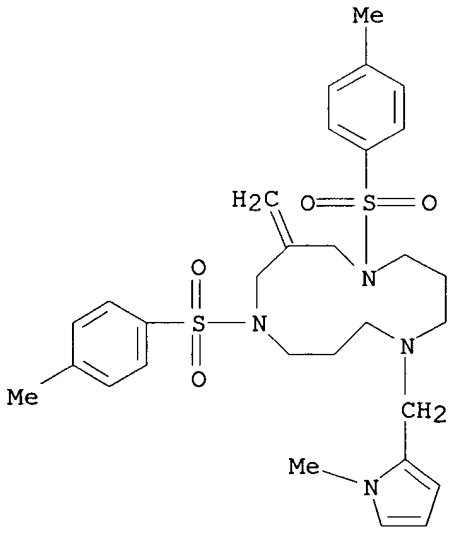
9-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT 182316-44-5P, CADA
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (methylene)bis[(methylphenyl)sulfonyl](benzyl)-1,5,9-triazacyclododecane (CADA) and study of its crystal and mol. structures)
RN 182316-44-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT 881693-35-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of (methylene)bis[(methylphenyl)sulfonyl](pyrazolylmethyl)-1,5,9-triazacyclododecane (CADA analog) and study of its crystal and mol. structures)
RN 881693-35-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-[(1-methyl-1H-pyrrol-2-yl)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

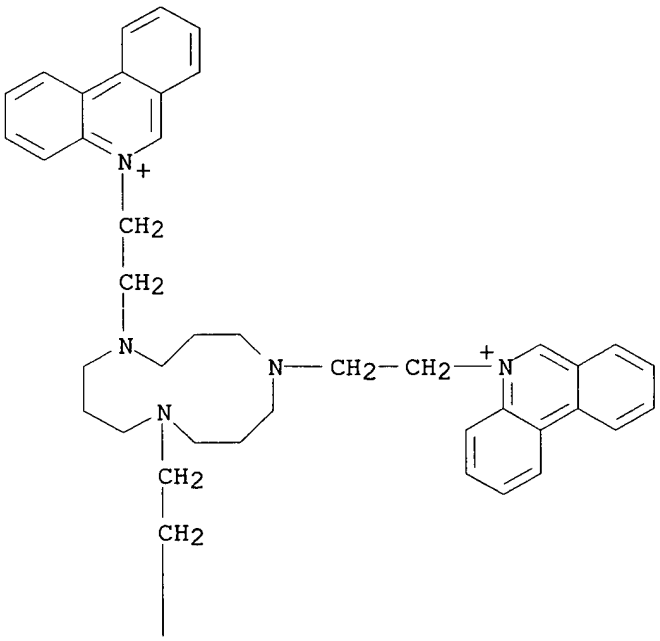
L80 ANSWER 4 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:704359 CAPLUS
DOCUMENT NUMBER: 143:326191
TITLE: An unusual substitution reaction directed by an intramolecular re-arrangement
AUTHOR(S): Parenty, Alexis D. C.; Smith, Louise V.; Cronin, Leroy
CORPORATE SOURCE: Department of Chemistry, University of Glasgow, Glasgow, G12 8QQ, UK
SOURCE: Tetrahedron (2005), 61(35), 8410-8418
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:326191

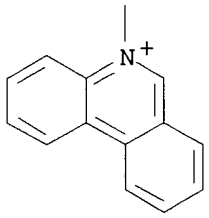
AB Secondary amines and thiols undertake a substitution reaction on the side chain of 2-bromoethylpyridinium derivs. directed by an intramol. rearrangement. Exptl. investigations strongly indicate that the reaction is initiated by an alpha addition of the nucleophile onto the iminium moiety of the N-heteroarom. cation, followed by a cyclization and an oxidative ring opening. This novel substitution process is able to occur with less reactive nucleophiles that would not undergo conventional substitution with isolated bromoethyl moieties.

IT 854516-25-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(rearrangement in the amination of fluoroethylphenanthridine)

RN 854516-25-9 CAPLUS
CN Phenanthridinium, 5,5',5''-(1,5,9-triazacyclododecane-1,5,9-triyltri-2,1-ethanediyl)tris-, tribromide (9CI) (CA INDEX NAME)

PAGE 1-A





● 3 Br^-

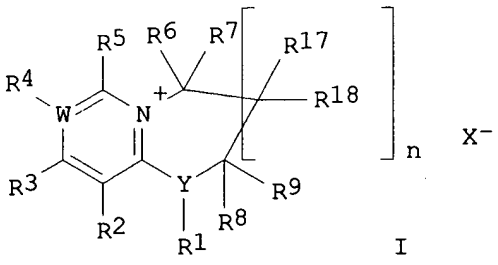
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 5 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:523454 CAPLUS
DOCUMENT NUMBER: 143:59981
TITLE: Preparation imidazophenanthridiniums and related compounds as anticancer agents
INVENTOR(S): Parenty, Alexis; Cronin, Leroy; Brown, Robert
PATENT ASSIGNEE(S): The University Court of the University of Glasgow, UK
SOURCE: PCT Int. Appl., 122 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

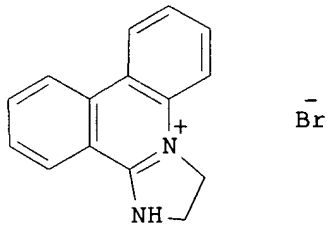
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005054241	A2	20050616	WO 2004-GB5004	20041126
WO 2005054241	A3	20050728		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1692130	A2	20060823	EP 2004-798693	20041126
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				

PRIORITY APPLN. INFO.: GB 2003-27524 A 20031126
WO 2004-GB5004 W 20041126

OTHER SOURCE(S): CASREACT 143:59981; MARPAT 143:59981
GI



I



II

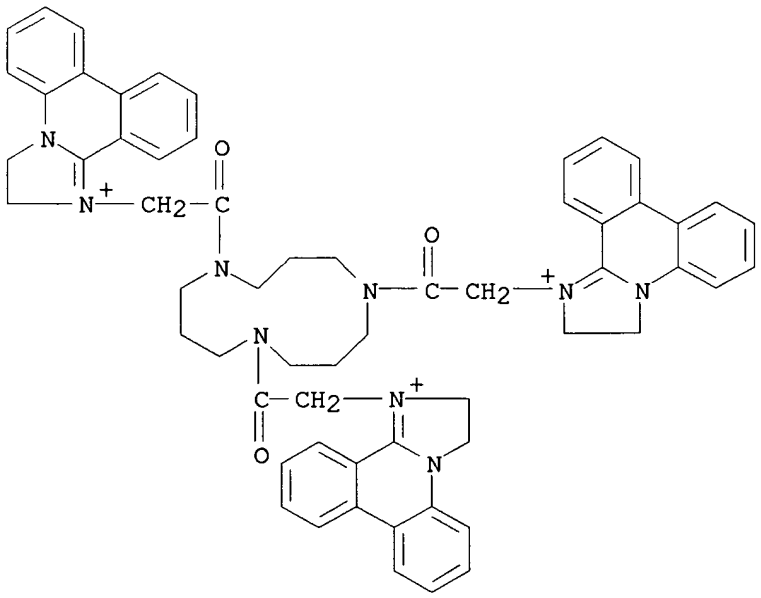
AB Title compds. I [n = 0-3; further details on n are given.; W = C, N; Y = N, O, S; R1 = H, (un)substituted alkyl, (un)substituted cycloalkyl, etc.; R2, R3, R4, R5 = halo, hydroxy, oxo, etc.; R6, R7 = H, halo, hydroxy, etc.; R8, R9 = H, halo, hydroxy, etc.; R17, R18 = H, halo, hydroxy, etc.; X = anion moiety] were prepared For example, bromoethylation of phenanthridine followed by treatment with 35% ammonia in water afforded compound II. In cytotoxicity assays, the IC50 value of compound II was 1.56 μM. Compds. I are claimed useful as anticancer agents, DNA binding agents, etc.

IT 854516-15-7P 854516-25-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation imidazophenanthridiniums and related compds. as anticancer agents)

RN 854516-15-7 CAPLUS

CN Imidazo[1,2-f]phenanthridinium, 1,1',1''-[1,5,9-triazacyclododecane-1,5,9-triyltris(2-oxo-2,1-ethanediyl)]tris[2,3-dihydro-, tribromide (9CI) (CA INDEX NAME)

PAGE 1-A

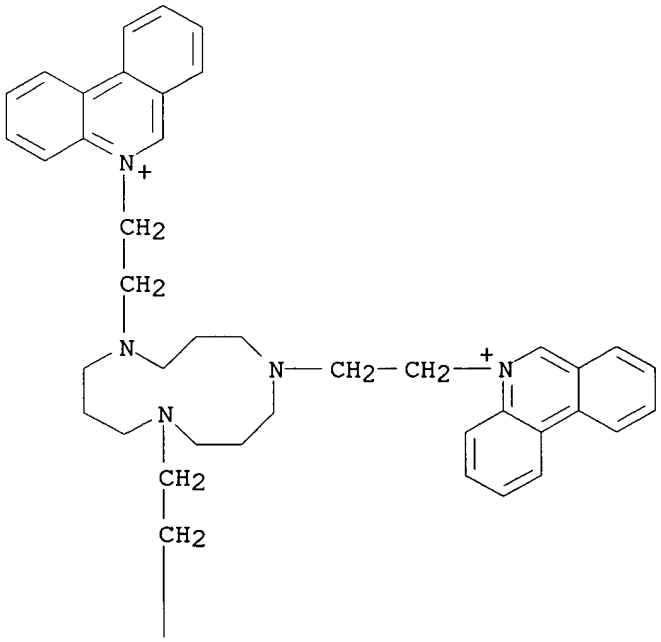


PAGE 2-A

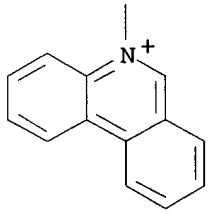
● 3 Br^-

RN 854516-25-9 CAPLUS
CN Phenanthridinium, 5,5',5''-(1,5,9-triazacyclododecane-1,5,9-triyltri-2,1-ethanediyl)tris-, tribromide (9CI) (CA INDEX NAME)

PAGE 1-A

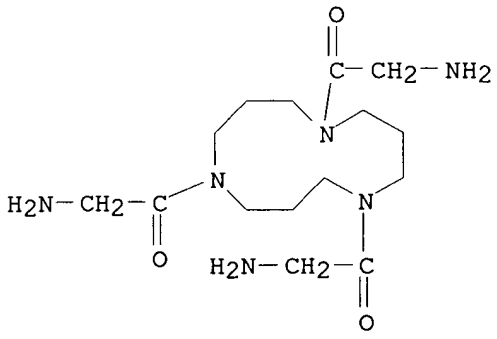


PAGE 2-A

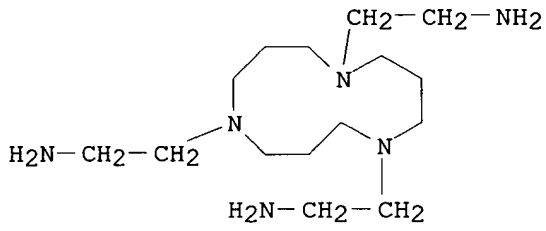


●3 Br^-

IT 854276-73-6 854276-74-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(spacer for trimer; preparation imidazophenanthridiniums and related compds. as anticancer agents)
RN 854276-73-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris(aminoacetyl)- (9CI) (CA INDEX NAME)



RN 854276-74-7 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triethanamine (9CI) (CA INDEX NAME)

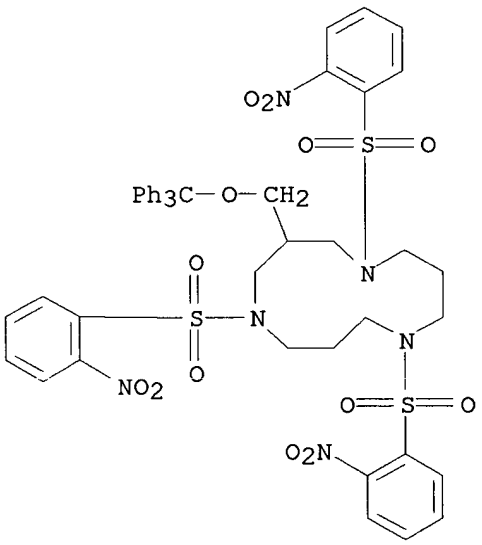


L30 ANSWER 6 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:461020 CAPLUS
DOCUMENT NUMBER: 143:153359
TITLE: Synthesis of azamacrocycles via a Mitsunobu reaction
AUTHOR(S): Hovinen, Jari; Sillanpaeae, Reijo
CORPORATE SOURCE: PerkinElmer Life and Analytical Sciences, Turku, FIN-20101, Finland
SOURCE: Tetrahedron Letters (2005), 46(25), 4387-4389
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:153359

AB Reaction of protected diethylenetriamine and 2-substituted propane-1,3-diols in dry THF in the presence of triphenylphosphine and diisopropyl azodicarboxylate gives the corresponding protected 9-substituted 1,4,7-triazacyclodecanes. The Mitsunobu reaction was also used in the preparation of 3-substituted 1,5,9-triazacyclododecanes and macrocyclic pyridine derivs.

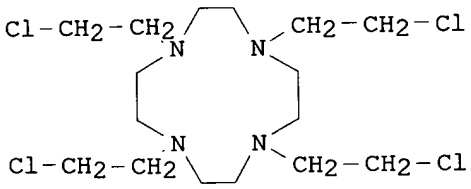
IT 859502-16-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of functionalized triazacyclodecanes, triazacyclododecanes and analogs via Mitsunobu reaction of protected dialkylenetriamines with diols)

RN 859502-16-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(2-nitrophenyl)sulfonyl]-3-[(triphenylmethoxy)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 7 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:202831 CAPLUS
DOCUMENT NUMBER: 142:456249
TITLE: Synthesis of novel DNA cross-linking antitumour agents based on polyazamacrocycles
AUTHOR(S): Parker, Laurie L.; Anderson, Fiona M.; O'Hare, C. Caroline; Lacy, Stephen M.; Bingham, John P.; Robins, David J.; Hartley, John A.
CORPORATE SOURCE: Department of Chemistry, University of Glasgow, Glasgow, G12 8QQ, UK
SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(7), 2389-2395
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:456249
GI

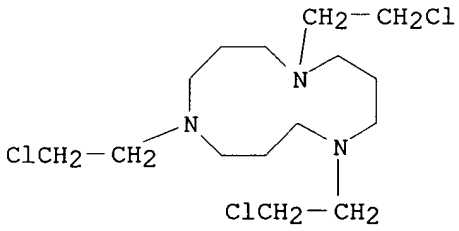


I

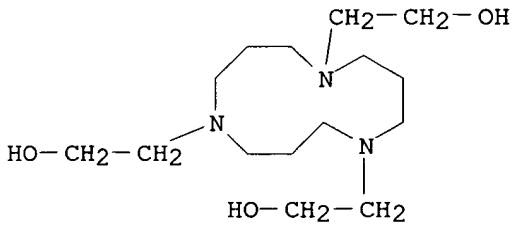
AB The authors are seeking to develop more effective alkylating agents as antitumor agents. In previous work conformationally restricted nitrogen mustards were synthesized containing piperidine or pyrrolidine rings. The free bases were designed to be bifunctional alkylating agents via aziridinium ion formation and the effects of varying the distances between the two alkylating sites were studied. Some efficient crosslinkers of naked DNA were prepared but few of these compds. exhibited significant cytotoxicity in human tumor cells in vitro. The authors have extended this work by making tri- and tetra-azamacrocyclic compds. containing two to four potential alkylating sites. Most of these compds. were powerful DNA alkylating agents and showed cytotoxicity (IC50 values 6-100 μM) comparable with chlorambucil (45 μM) and melphalan (8.5 μM). In particular the cyclen derivative I was more than 104 times more effective at crosslinking DNA (XL50 « 10 nM) than chlorambucil (XL50 100 μM), and showed significant cytotoxicity in human tumor cells in vitro.

IT 850894-95-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of novel DNA crosslinking antitumor agents based on polyazamacrocycles)

RN 850894-95-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris(2-chloroethyl)- (9CI) (CA INDEX NAME)



IT 850895-04-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of novel DNA crosslinking antitumor agents based on polyazamacrocycles)
RN 850895-04-4 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triethanol (9CI) (CA INDEX NAME)



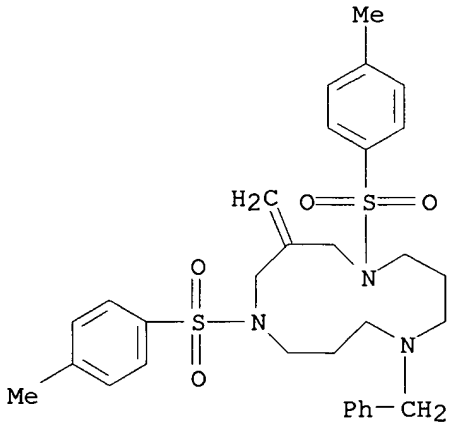
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 8 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:1079564 CAPLUS
DOCUMENT NUMBER: 142:232412
TITLE: CADA, a novel CD4-targeted HIV inhibitor, is synergistic with various anti-HIV drugs in vitro
AUTHOR(S): Vermeire, Kurt; Princen, Katrien; Hatse, Sigrid; de Clercq, Erik; Dey, Kaka; Bell, Thomas W.; Schols, Dominique
CORPORATE SOURCE: Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.
SOURCE: AIDS (London, United Kingdom) (2004), 18(16), 2115-2125
CODEN: AIDSET; ISSN: 0269-9370
PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Objective: To evaluate the anti-HIV-1 activity of the cyclotriazadisulfonamide CADA against primary isolates in vitro and the combination of CADA with approved anti-HIV drugs for potential synergy. Methods: Peripheral blood mononuclear cells (PBMC) were treated with CADA and infected with 16 different clin. isolates. After 8 days of infection, the median inhibitory concentration (IC50) was calculated from the p24 viral antigen content in the supernatant. MT-4 cells were infected with HIV-1NL4.3 and then cultured with CADA or other antiretroviral drugs (i.e., several reverse transcriptase, protease and entry inhibitors), alone and in combination. After 4 days, IC50 was determined for the various drugs in replicate assays. Anal. of combined effects was performed using the median effect principle (CalcuSyn; Biosoft). Results: The entry inhibitor CADA exerted a potent and consistent anti-HIV-1 activity against a wide range of R5, R5/X4 and X4 primary isolates in PBMC. From the two-drug studies, combination indexes showed synergy between CADA and reverse transcriptase inhibitors (zidovudine, stavudine, lamivudine, zalcitabine, didanosine, abacavir, tenofovir, nevirapine, delavirdine and efavirenz), and protease inhibitors (lopinavir, saquinavir, indinavir, nelfinavir, amprenavir and ritonavir). In addition, the combination of CADA with the gp41 fusion inhibitor T-20 (enfuvirtide), the CXCR4 antagonist AMD3100 and the gp120-specific interacting plant lectins from Galanthus nivalis (GNA) and Hippeastrum hybrid (HHA) also resulted in a synergistic inhibition. Conclusions: Compds. that can specifically downmodulate the CD4 receptor in PBMC have broad-spectrum anti-HIV activity against primary isolates and act synergistically when used in conjunction with currently available antiretroviral drugs. They deserve further study as potential candidate anti-HIV drugs.

IT 182316-44-5, CADA
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(CD4-downmodulating compound CADA with potent anti-HIV-1 activity against R5, R5/X4 and X4 primary isolates in PBMC and showed favorable in vitro interaction and synergistic action with antiretroviral agent like RT, protease, entry inhibitor)

RN 182316-44-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



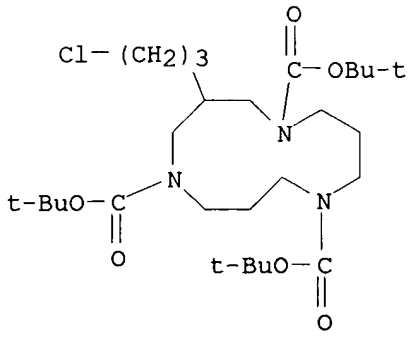
REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 9 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:996287 CAPLUS
DOCUMENT NUMBER: 140:235998
TITLE: Preparation of Aza-Crown-Functionalized 2'-O-Methyl Oligoribonucleotides, Potential Artificial RNases
AUTHOR(S): Niittymaeki, Teija; Kaukinen, Ulla; Virta, Pasi; Mikkola, Satu; Loennberg, Harri
CORPORATE SOURCE: Department of Chemistry, University of Turku, Turku, FIN-20014, Finland
SOURCE: Bioconjugate Chemistry (2004), 15(1), 174-184
CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

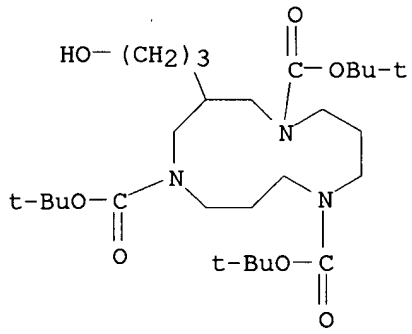
AB An improved synthesis for 3-(3-aminopropyl)- and 3-(3-mercaptopropyl)-1,5,9-triazacyclododecane has been developed and alternative methods for their conjugation to oligonucleotides have been described. Accordingly, the 3-aminopropyl aza-crown and its N-(3-aminopropanoyl)-3-aminopropyl analog have been tethered to the 3'-terminus of a 2'-O-methyloligoribonucleotide by aminolytic cleavage of the thio-ester linker utilized for the chain assembly. Studies on a monomeric model compound verify that the reaction proceeds solely by the attack of the primary amino group. 5'-Conjugation has been achieved by introducing a 2-benzylthio-2-oxoethyl group to the 5'-terminus as a phosphoramidite reagent and cleaving the thioester bond with the 3-aminopropyl aza-crown. For intrachain conjugation, a phosphoramidite reagent derived from 1-deoxy-1-(2-benzylthio-2-oxoethyl)-β-D-erythro-pentofuranose has been inserted in a desired position within the chain and subjected to on-support aminolysis with the 3-aminopropyl aza-crown or its N-(3-aminopropanoyl)-3-aminopropyl and N-(6-aminohexanoyl)-3-aminopropyl analogs. The 3-mercaptopropyl-derivatized aza-crown has been tethered by a disulfide bond to a 3'-(3-mercaptoalkyl)phosphate-tailed oligonucleotide. The 3'- and intrachain-tethered conjugates have been shown to cleave as their Zn(II) chelate complementary oligoribonucleotide sequences.

IT 663198-88-7P 663198-89-8P 663198-90-1P
663198-91-2P 663198-93-4P 663198-94-5P
663198-96-7P 663198-97-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aza-crown-functionalized 2'-O-Me oligoribonucleotides as potential artificial RNases)

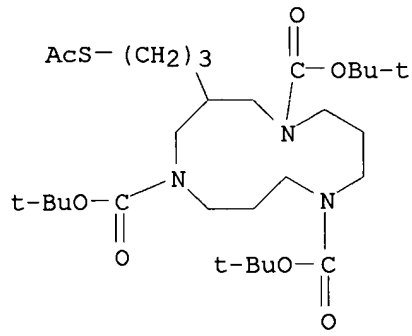
RN 663198-88-7 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-(3-chloropropyl)-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



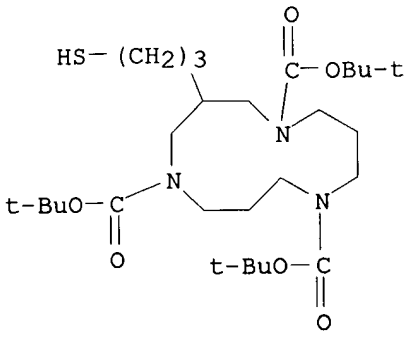
RN 663198-89-8 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-(3-hydroxypropyl)-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



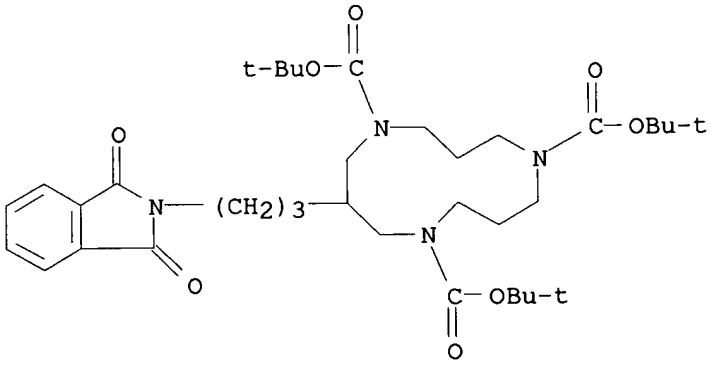
RN 663198-90-1 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-[3-(acetylthio)propyl]-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



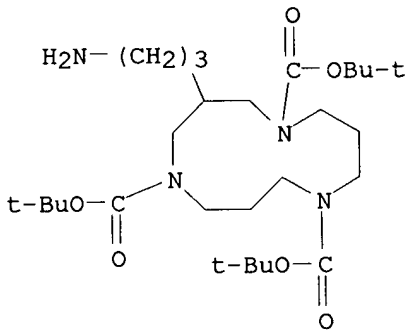
RN 663198-91-2 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-(3-mercaptopropyl)-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



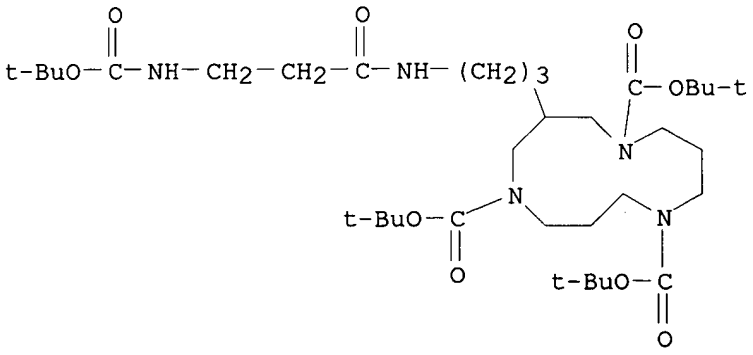
RN 663198-93-4 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



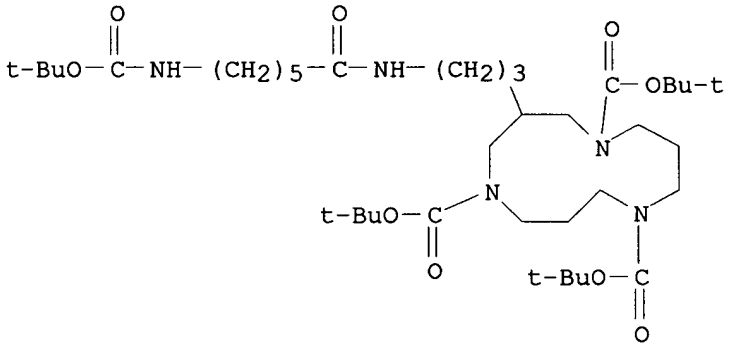
RN 663198-94-5 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-(3-aminopropyl)-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 663198-96-7 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-[3-[[3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-oxopropyl]amino]propyl]-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 663198-97-8 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, 3-[3-[[6-[[(1,1-dimethylethoxy)carbonyl]amino]-1-oxohexyl]amino]propyl]-, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 10 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:727508 CAPLUS
DOCUMENT NUMBER: 139:350441
TITLE: Syntheses, Conformations, and Basicities of Bicyclic Triamines
AUTHOR(S): Bell, Thomas W.; Choi, Heung-Jin; Harte, William; Drew, Michael G. B.
CORPORATE SOURCE: Department of Chemistry, University of Nevada, Reno, NV, 89557-0020, USA
SOURCE: Journal of the American Chemical Society (2003), 125(40), 12196-12210
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:350441
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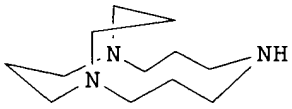
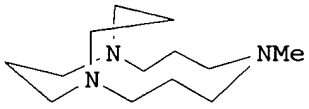
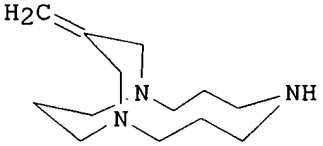


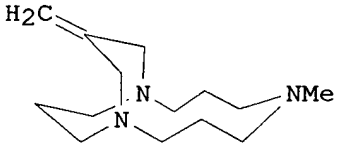
XII



XIII



XV



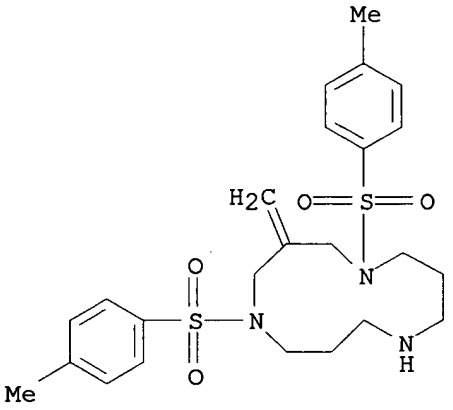
XVI

AB The multistep syntheses of several bicyclic triamines are described, all of which have an imbedded 1,5,9-triazacyclododecane ring. In 1,5,9-triazabicyclo[7.3.3]pentadecanes 12, 13, 15, and 16, (XII, XIII, XV, and XVI, resp.) two nitrogens are bridged by three carbons. The monoprotonated forms of these triamines are highly stabilized by a hydrogen-bonded network involving the bridge and both bridgehead nitrogens, producing a difference of more than 8 pKa units in acidities of their monoprotonated and diprotonated forms. The one- and zero-carbon bridges in 1,5,9-triazabicyclo[9.1.1]tridecane and 7-methyl-1,5,9-triazabicyclo[5.5.0]dodecane do not enhance the stabilities of their monoprotonated forms. X-ray crystal structures and computational studies of 12·HI and 16·HI reveal similar, but somewhat weaker, hydrogen-bonded networks, relative to 15·HI. The activation free energies for conformational inversion of 13·HI (14.4 ± 0.2 kcal/mol), 16·HI (15.0 ± 0.1 kcal/mol) and 16 (8.8 ± 0.3 kcal/mol) were measured by variable-temperature 1H and 13C NMR spectroscopy. These exptl. barriers give an estimate of 6.2 kcal/mol for the strength of the bifurcated hydrogen bond between the bridge nitrogen and cavity proton in 16·HI. Computational studies support the hypothesis that N-inversion occurs in an open conformation, leading to an estimate of 10.32 kcal/mol for the enthalpy of the bifurcated hydrogen bond in 16·HI in the gas phase. Safety: explosion hazard; air must be completely replaced by H2 in Parr apparatus before hydrogenation of bis(2-cyanoethyl)benzylamine.

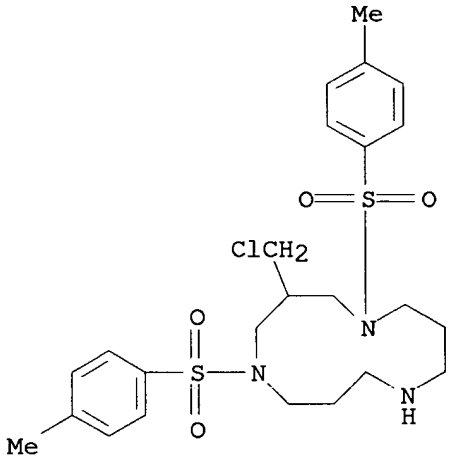
IT 182316-06-9P 182316-12-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(attempted cyclization; syntheses, conformations, and basicities of bicyclic triamines containing embedded 1,5,9-triazacyclododecane ring)

RN 182316-06-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

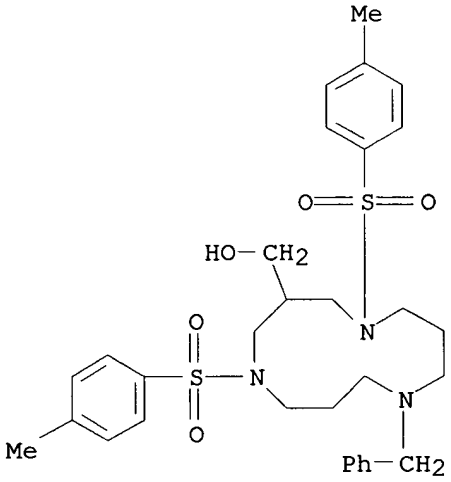


RN 182316-12-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



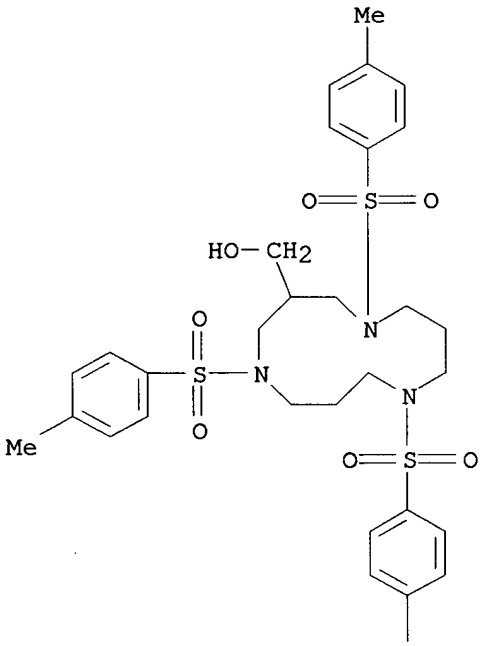
IT 182316-08-1P 182316-17-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(chlorination; syntheses, conformations, and basicities of bicyclic triamines containing embedded 1,5,9-triazacyclododecane ring)

RN 182316-08-1 CAPLUS
CN 1,5,9-Triazacyclododecane-3-methanol, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



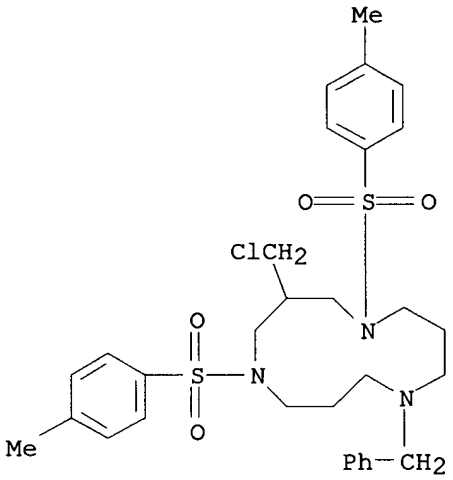
RN 182316-17-2 CAPLUS
CN 1,5,9-Triazacyclododecane-3-methanol, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

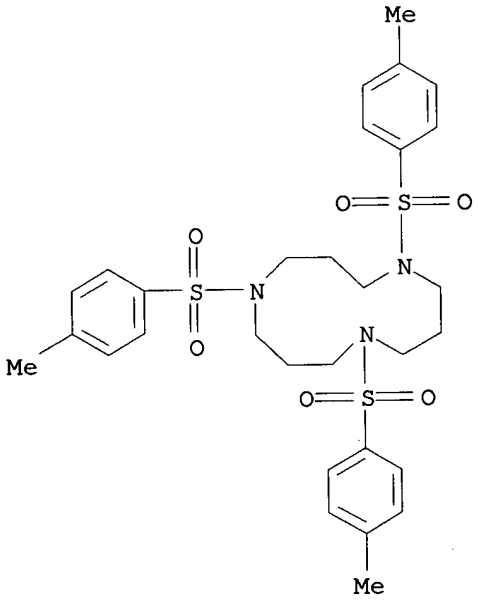


PAGE 2-A

IT 182316-10-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(deprotection; syntheses, conformations, and basicities of bicyclic triamines containing embedded 1,5,9-triazacyclododecane ring)
RN 182316-10-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

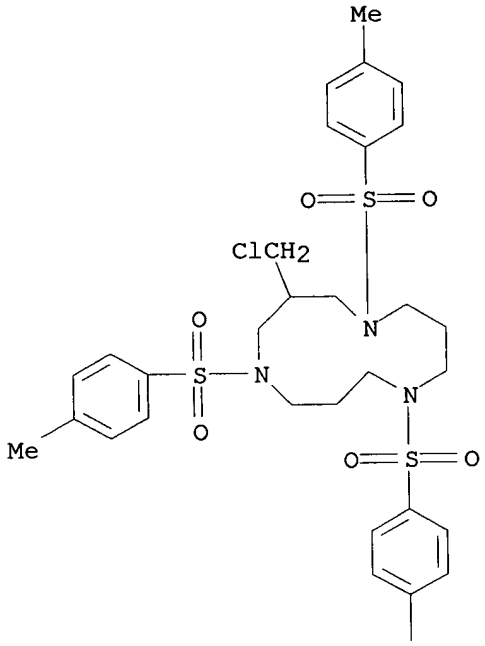


IT 35980-67-7P 182316-19-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(detosylation; syntheses, conformations, and basicities of bicyclic triamines containing embedded 1,5,9-triazacyclododecane ring)
RN 35980-67-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 182316-19-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

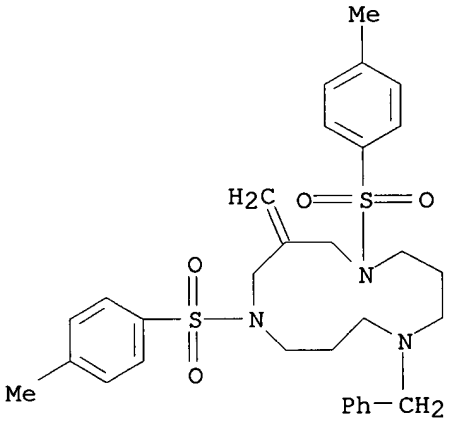
PAGE 1-A



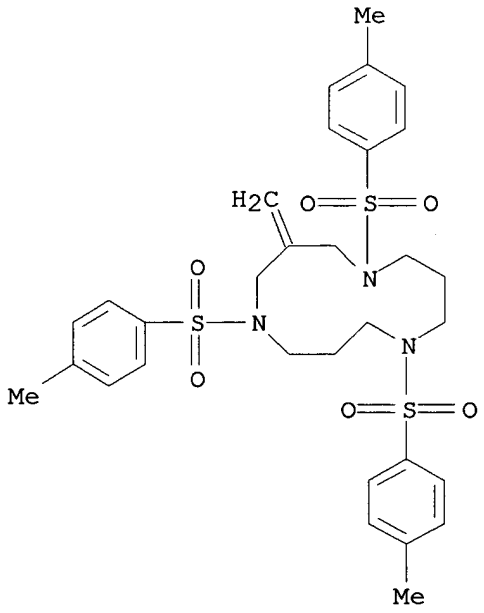
PAGE 2-A

Me

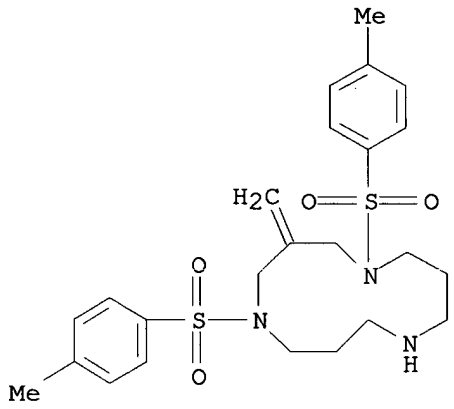
IT 182316-44-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(hydroboration/oxidation and deprotection; syntheses, conformations, and basicities of bicyclic triamines containing embedded 1,5,9-triazacyclododecane ring)
RN 182316-44-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT 182316-15-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(hydroboration/oxidation; syntheses, conformations, and basicities of bicyclic triamines containing embedded 1,5,9-triazacyclododecane ring)
RN 182316-15-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

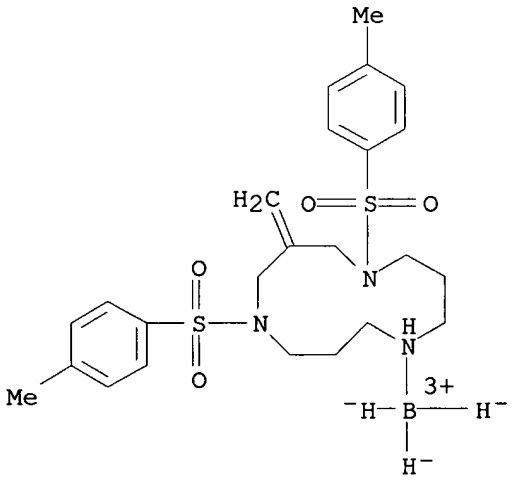


IT 392287-04-6P 618097-39-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(syntheses, conformations, and basicities of bicyclic triamines containing embedded 1,5,9-triazacyclododecane ring)
RN 392287-04-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 618097-39-5 CAPLUS
CN Boron, trihydro[3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododecane-κN9]-, (T-4)- (9CI) (CA INDEX NAME)



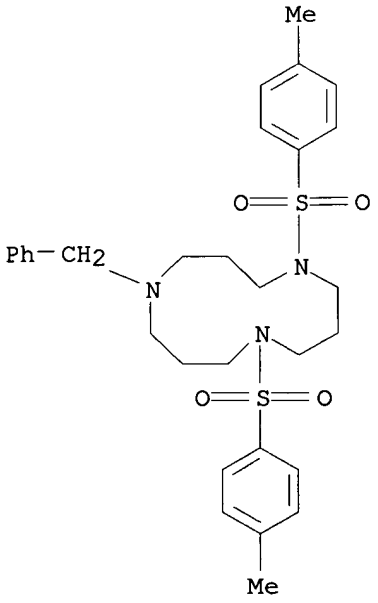
REFERENCE COUNT: 94 THERE ARE 94 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 11 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:3477 CAPLUS
DOCUMENT NUMBER: 139:30160
TITLE: The anti-HIV potency of cyclotriazadisulfonamide analogs is directly correlated with their ability to down-modulate the CD4 receptor
AUTHOR(S): Vermeire, Kurt; Bell, Thomas W.; Choi, Heung-Jin; Jin, Qi; Samala, Meinrado F.; Sodoma, Andrej; De Clercq, Erik; Schols, Dominique
CORPORATE SOURCE: Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, Belg.
SOURCE: Molecular Pharmacology (2003), 63(1), 203-210
CODEN: MOPMA3; ISSN: 0026-895X
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

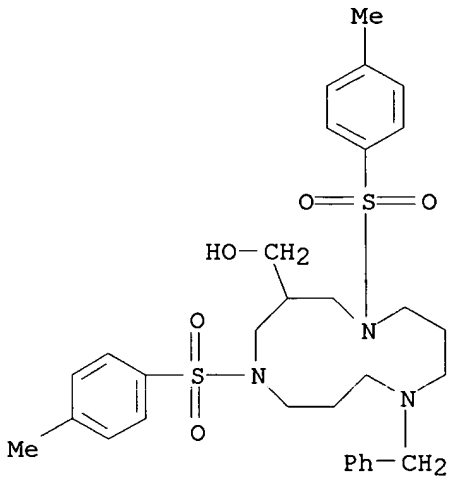
AB 9-Benzyl-3-methylene-1,5-di-p-toluenesulfonyl-1,5,9-triazacyclododecane (CADA) has been identified as a novel antiviral lead compound with significant anti-human immunodeficiency virus and anti-human herpesvirus 7 activity. Surprisingly, this compound selectively decreased the expression of the CD4 glycoprotein, the primary receptor needed for the entry of both viruses. Herein, we describe the CD4 down-modulating and antiviral potencies of more than 25 CADA derivs. Flow cytometric evaluation of cellular CD4 receptor expression in T cells demonstrated the specific CD4 down-modulating capacity of the CADA derivs., with IC50 values similar to those obtained in the antiviral assays. The close correlation observed between the CD4 down-regulating and anti-HIV potencies of the CADA derivs. further points to CD4 receptor down-modulation as the primary mode of antiviral action for this group of compds.

IT 164913-15-9 182316-08-1 182316-10-5
182316-15-0 182316-20-7 182316-30-9
182316-34-3 182316-44-5 471866-86-1
471866-87-2 471866-89-4 471866-90-7
471866-91-8 471866-92-9 471866-93-0
471866-94-1 471866-95-2 471866-96-3
471866-97-4 471866-98-5 471866-99-6
471867-00-2 471867-02-4 471867-03-5
471867-04-6 471867-05-7 471867-06-8
544430-76-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(the anti-HIV potency of cyclotriazadisulfonamide analogs is directly correlated with their ability to down-modulate the CD4 receptor)

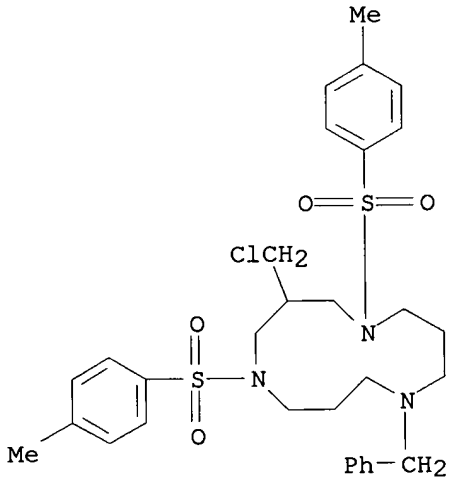
RN 164913-15-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



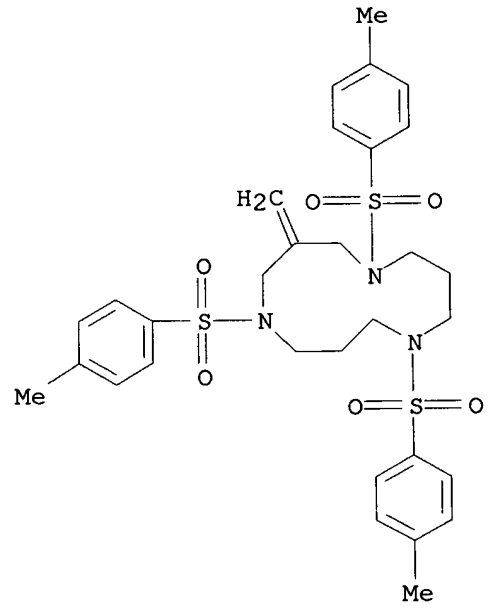
RN 182316-08-1 CAPLUS
CN 1,5,9-Triazacyclododecane-3-methanol, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



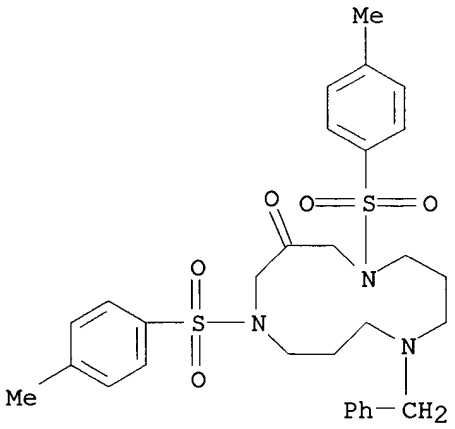
RN 182316-10-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



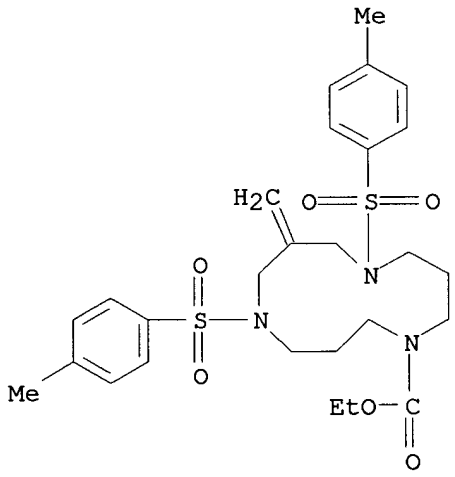
RN 182316-15-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



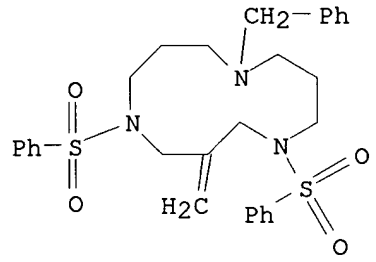
RN 182316-20-7 CAPLUS
CN 1,5,9-Triazacyclododecan-3-one, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



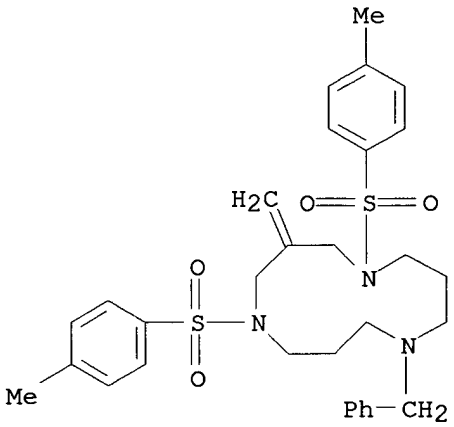
RN 182316-30-9 CAPLUS
CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)



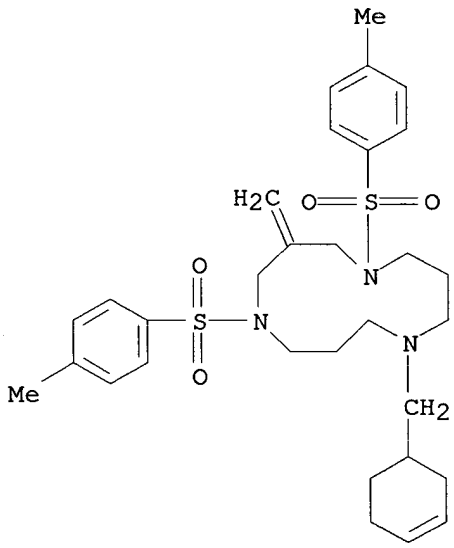
RN 182316-34-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-9-(phenylmethyl)-1,5-bis(phenylsulfonyl)- (9CI) (CA INDEX NAME)



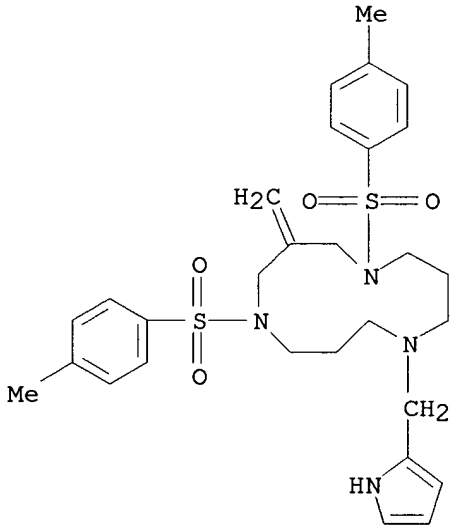
RN 182316-44-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 471866-86-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(3-cyclohexen-1-ylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 471866-87-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(1H-pyrrol-2-ylmethyl)- (9CI) (CA INDEX NAME)



RN 471866-89-4 CAPLUS
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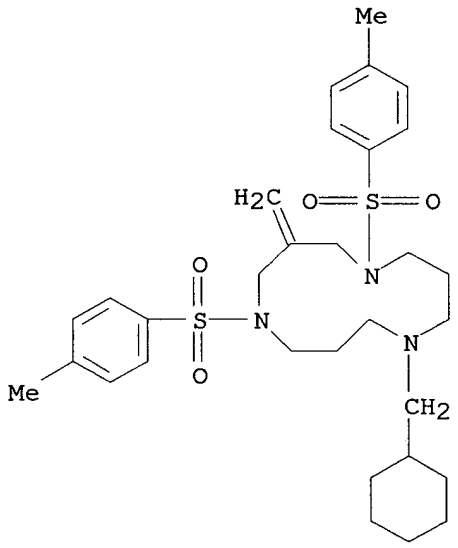
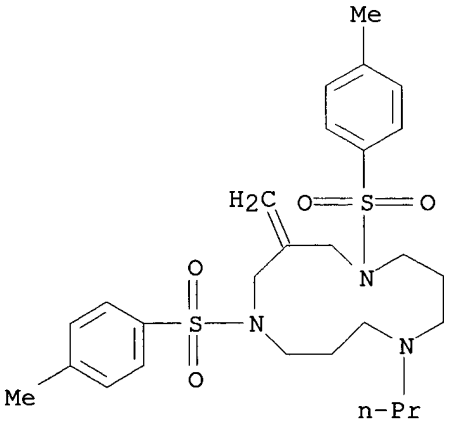
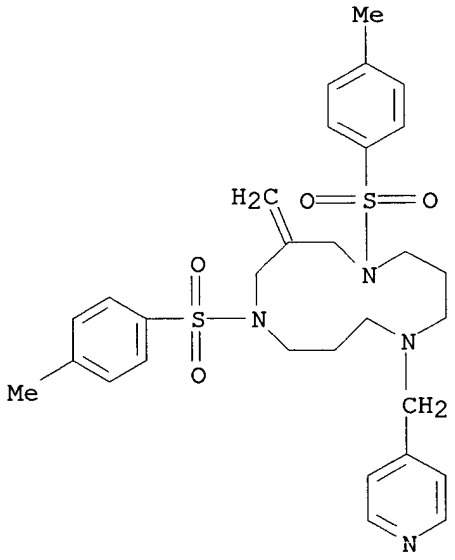


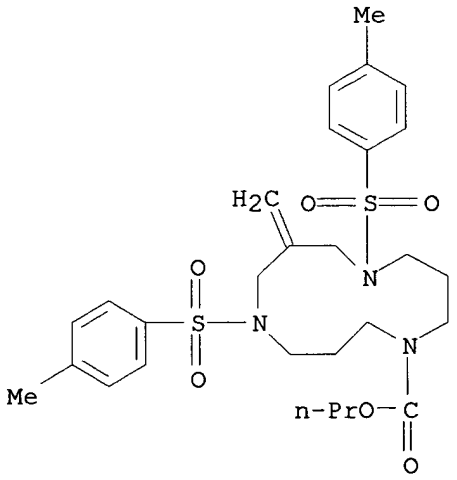
RN 471866-90-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-propyl- (9CI) (CA INDEX NAME)



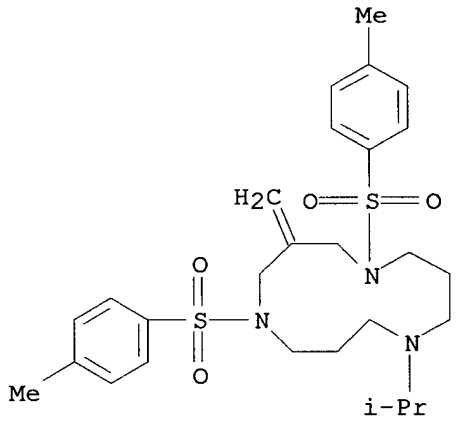
RN 471866-91-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



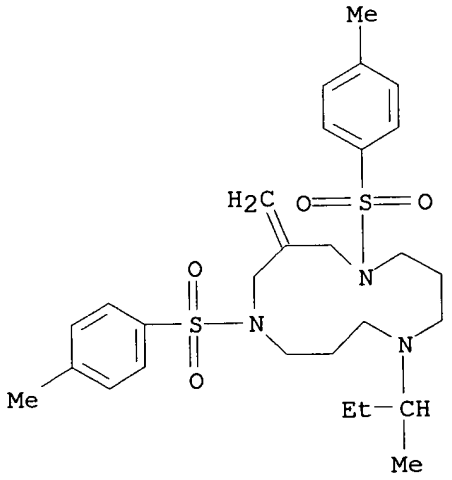
RN 471866-92-9 CAPLUS
CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, propyl ester (9CI) (CA INDEX NAME)



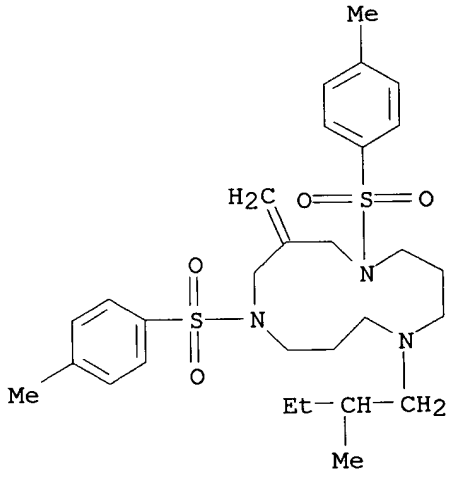
RN 471866-93-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-9-(1-methylethyl)-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



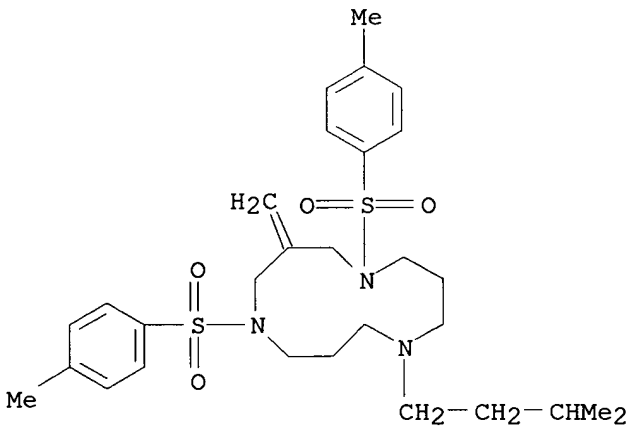
RN 471866-94-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(1-methylpropyl)- (9CI) (CA INDEX NAME)



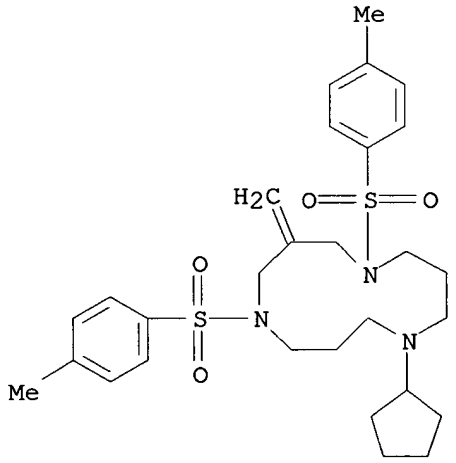
RN 471866-95-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(2-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



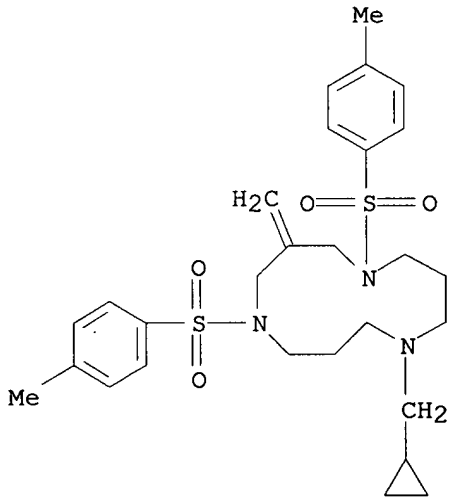
RN 471866-96-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(3-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



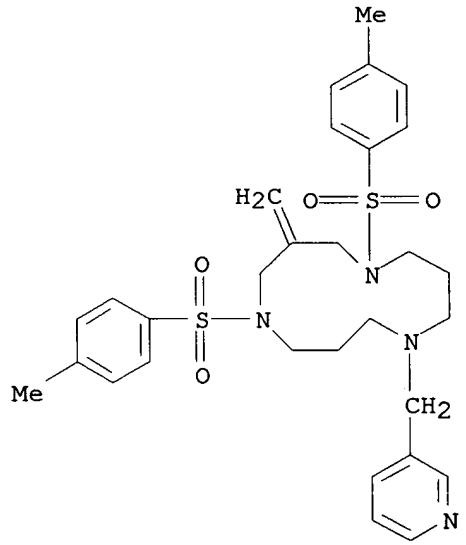
RN 471866-97-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-cyclopentyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



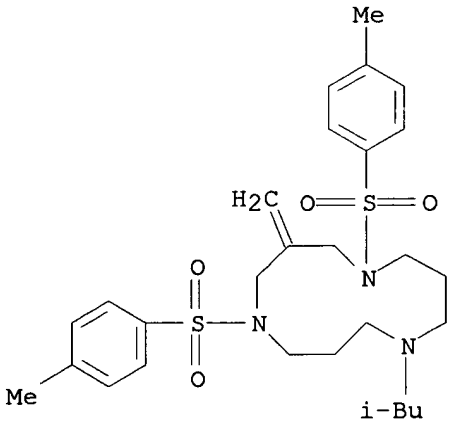
RN 471866-98-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(cyclopropylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



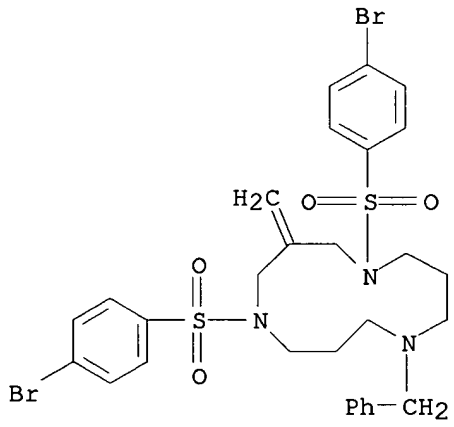
RN 471866-99-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)



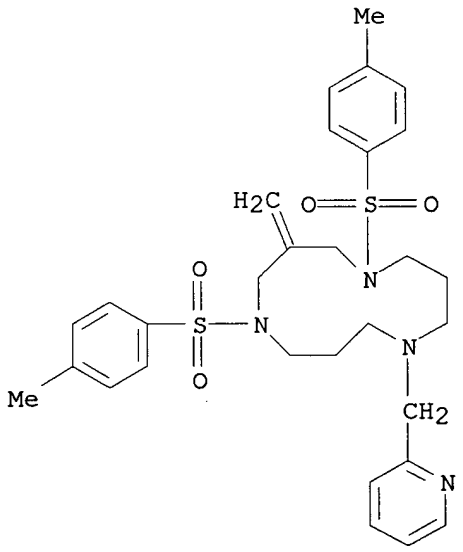
RN 471867-00-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-methylpropyl)- (9CI) (CA INDEX NAME)



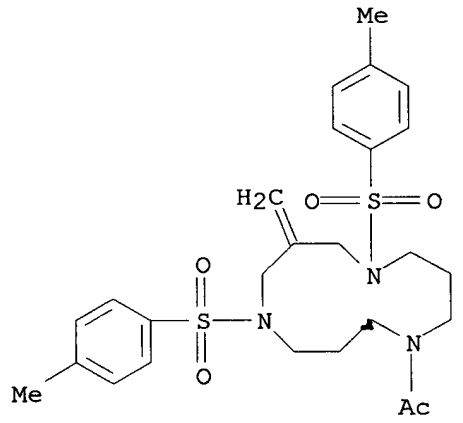
RN 471867-02-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-bromophenyl)sulfonyl]-3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



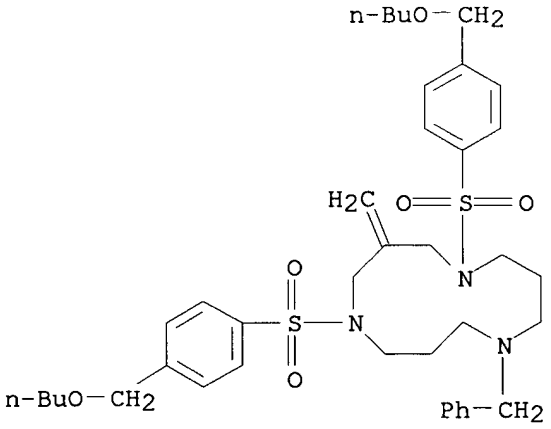
RN 471867-03-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



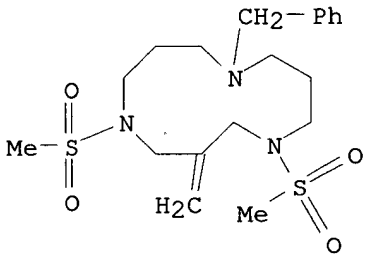
RN 471867-04-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-acetyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



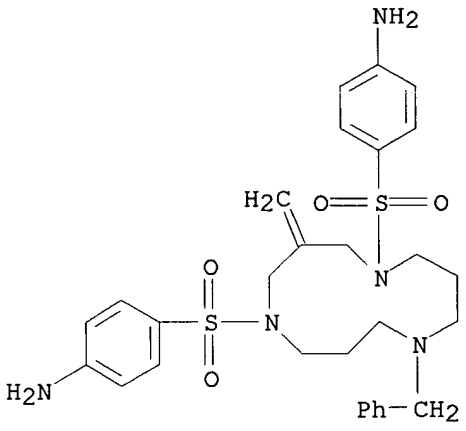
RN 471867-05-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[[4-(butoxymethyl)phenyl]sulfonyl]-3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 471867-06-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis(methylsulfonyl)-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 544430-76-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-aminophenyl)sulfonyl]-3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



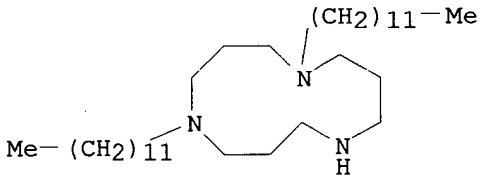
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 12 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:880548 CAPLUS
DOCUMENT NUMBER: 138:140271
TITLE: Strongly basic macrocyclic triamines, 1,5,9-triazacyclododecanes for solvent extraction of gold(I) cyanide
AUTHOR(S): Choi, Heung-Jin; Bae, Yoon-Kyung; Kang, Seok-Chan; Park, Yeon Sil; Park, Joon Won; Kim, Woong-Il; Bell, Thomas W.
CORPORATE SOURCE: Department of Industrial Chemistry, Kyungpook National University, Taegu, 702-701, S. Korea
SOURCE: Tetrahedron Letters (2002), 43(51), 9385-9389
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

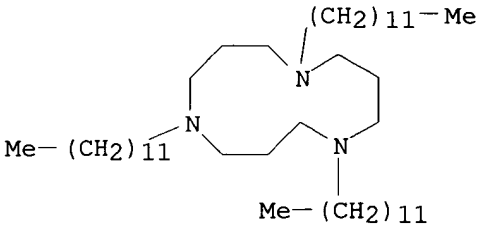
AB Solvent extraction of gold(I) dicyanide anion from alkaline gold(I) cyanide solution by using unusually basic amine extractants was conducted. The 1,5,9-Triazacyclododecane (IV) is known as an unusually basic macrocyclic amine having pKa = 12.3-12.7 and is thus a candidate as a basic amine extractant. Three lipophilic derivs. of IV expected to stay in the organic phase during gold solvent extraction were synthesized. N-Dodecyl-1,5,9-triazacyclododecane (III) was prepared from 1,5,9-triazacyclododecane-2,4-dione (I) by N-alkylation with n-dodecyl iodide and then reduction with BH3-THF. N,N'-Didodecyl-1,5,9-triazacyclododecane (V) and N,N',N''-tridodecyl-1,5,9-triazacyclododecane (VI) were efficiently synthesized by selective di-alkylation of IV with n-dodecyl iodide, and by reductive alkylation of IV with n-dodecanol, resp. Extractants III and VI extracted 50% of the metal at pH 10.5, which is the min. value required for practical application.

IT 494769-64-1 494769-65-2
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); PROC (Process)
(strongly basic macrocyclic triamines as extractants for solvent extraction of gold(I) cyanide)

RN 494769-64-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-didodecyl- (9CI) (CA INDEX NAME)



RN 494769-65-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tridodecyl- (9CI) (CA INDEX NAME)

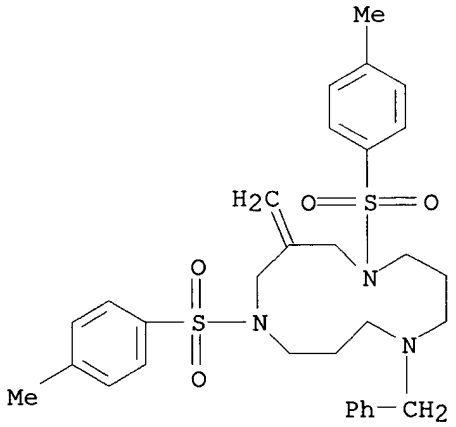


REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 13 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:851418 CAPLUS
DOCUMENT NUMBER: 138:395471
TITLE: CADA Inhibits Human Immunodeficiency Virus and Human Herpesvirus 7 Replication by Down-modulation of the Cellular CD4 Receptor
AUTHOR(S): Vermeire, Kurt; Zhang, Ying; Princen, Katrien; Hatse, Sigrid; Samala, Meinrado F.; Dey, Kaka; Choi, Heung-Jin; Ahn, Youngmi; Sodoma, Andrej; Snoeck, Robert; Andrei, Graciela; De Clercq, Erik; Bell, Thomas W.; Schols, Dominique
CORPORATE SOURCE: Rega Institute for Medical Research, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.
SOURCE: Virology (2002), 302(2), 342-353
CODEN: VIRLAX; ISSN: 0042-6822
PUBLISHER: Elsevier Science
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The novel antiviral agent cyclotriazadisulfonamide (CADA) inhibited human immunodeficiency virus (HIV) (IC50, 0.3-3.2 μM) and human herpesvirus 7 (HHV-7) infection (IC50, 0.3-1.5 μM) in T-cell lines and PBMCs. When T-cells were pretreated with CADA for 24 h, they became markedly protected from viral infection. Flow cytometric anal. revealed a significant decrease in the expression of the CD4 glycoprotein, the primary receptor needed for entry of both viruses. Moreover, the antiviral activity of CADA correlated with its ability to down-modulate the CD4 receptor. CADA did not alter the expression of any other cellular receptor (or HIV coreceptor) examined Time course expts. showed that CD4 down-modulation by CADA differs in mechanism from the effects of aurintricarboxylic acid, which binds directly to CD4, and phorbol myristate acetate, which activates protein kinase C. Further anal. of CD4 mRNA levels suggested that CADA was not involved in the regulation of CD4 expression at a transcriptional level, but very likely at (post) translational levels. This unique mechanism of action makes CADA an important lead in developing new drugs for treatment of AIDS, autoimmune diseases, and inflammatory disorders.

IT 392287-03-5
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(cyclotriazadisulfonamide (CADA) inhibits human immunodeficiency virus and human herpesvirus 7 replication by down-modulation of cellular CD4 receptor)
RN 392287-03-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

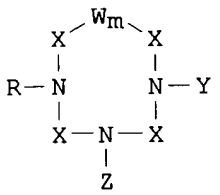
REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

applicant

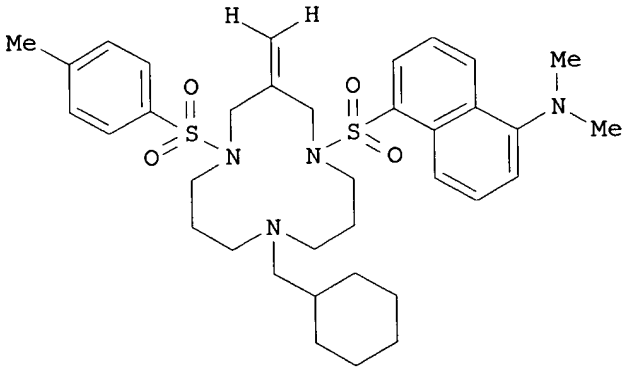
L30 ANSWER 14 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:793364 CAPLUS
DOCUMENT NUMBER: 137:304743
TITLE: Macrocyclic triaza compounds as immunoregulatory agents
INVENTOR(S): Bell, Thomas W.; Schols, Dominique; Dey, Kaka; Vermeire, Kurt
PATENT ASSIGNEE(S): University and Community College System of Nevada on Behalf of the University of Nevada, Reno, USA
SOURCE: PCT Int. Appl., 70 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002080856	A2	20021017	WO 2002-US11223		20020408
WO 2002080856	A3	20040318			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2002303293	A1	20021021	AU 2002-303293		20020408
US 2004220164	A1	20041104	US 2003-680076		20031006
PRIORITY APPLN. INFO.:			US 2001-282212P	P	20010406
			WO 2002-US11223	W	20020408

OTHER SOURCE(S): MARPAT 137:304743
GI



I



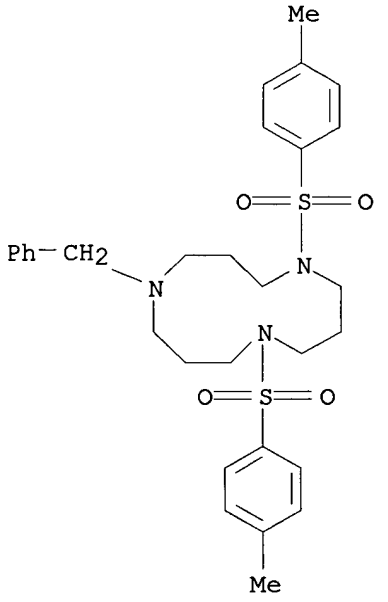
II

AB Title compds. I [W = a bridge carbon which is unsubstituted or is bonded directly or indirectly to one or two polar or non-polar side group substituents; R and Y independently = (un)substituted aryl, alkyl or alkenyl attached through an optional linker group; Z = H, (un)substituted aryl, alkyl or alkenyl attached through a linking group; X = Ca-d which represents carbon bridges, preferably alkylene bridges, between nitrogens, the length of which is defined by the subscripts a-d, the bridges may be optionally substituted and saturated or unsatd.; a and d independently = 0-10; b and c independently = 1-10; m = 0-3], which down-regulate CD4 expression for use in the treatment of autoimmune diseases and inflammatory diseases or conditions, are disclosed. In a specific embodiment, the invention provides certain naphthalene substituted triaza macrocycles which exhibit high activity for down regulation of CD4 expression. In particular, triaza macrocycles having dansyl groups, e.g., II, are provided for use in pharmaceutical compns. II possessed an IC50 (μg/mL) value of 0.41 in assays to determine CD4 down-modulating activity in MT-4 cells.

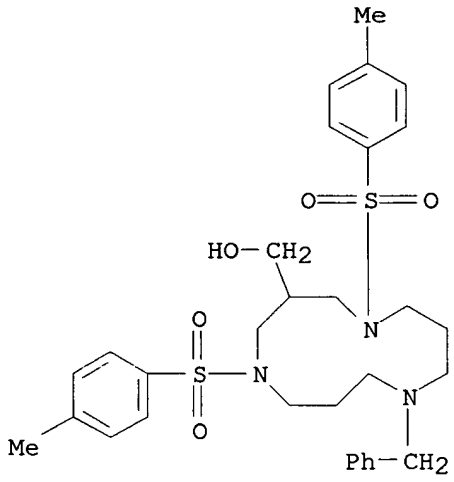
IT 164913-15-9 182316-08-1 182316-10-5
182316-15-0 182316-20-7 182316-30-9
182316-44-5 392287-03-5 471866-86-1
471866-87-2 471866-89-4 471866-90-7
471866-91-8 471866-92-9 471866-93-0
471866-94-1 471866-95-2 471866-96-3
471866-97-4 471866-98-5 471866-99-6
471867-00-2 471867-01-3 471867-02-4
471867-03-5 471867-04-6 471867-05-7
471867-06-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(evaluation of triazamacrocycles as immunoregulatory agents with CD4 down-modulating activity)

RN 164913-15-9 CAPLUS

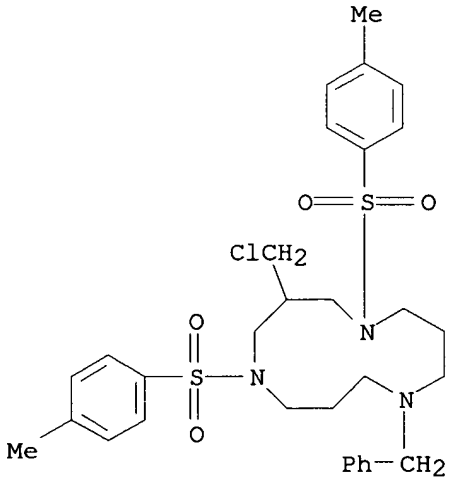
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



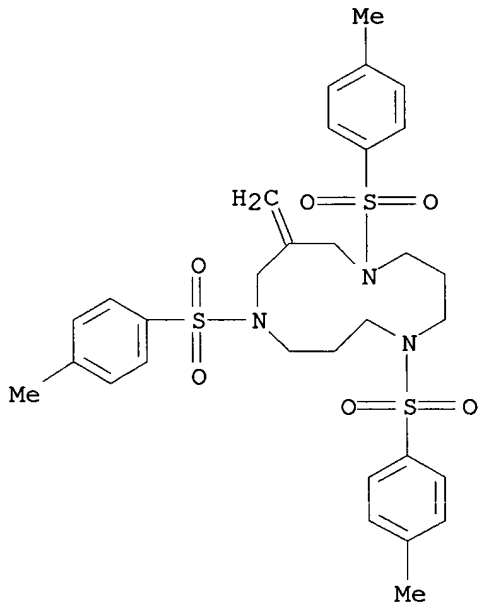
RN 182316-08-1 CAPLUS
CN 1,5,9-Triazacyclododecane-3-methanol, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



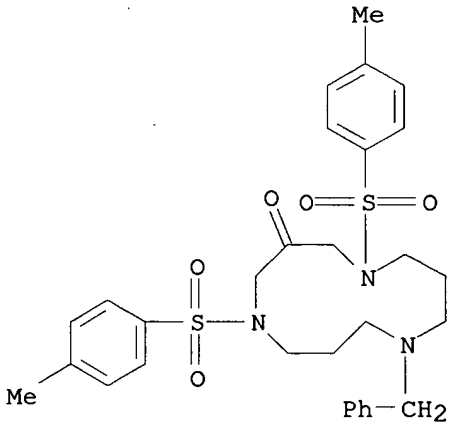
RN 182316-10-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



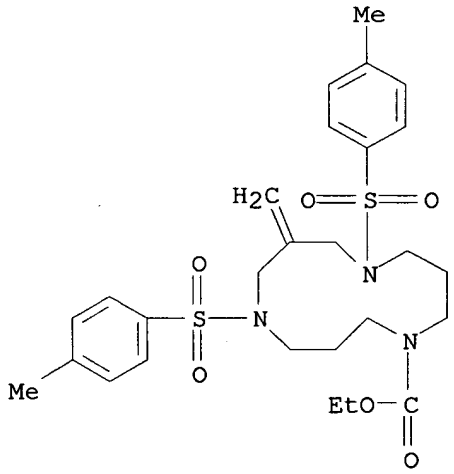
RN 182316-15-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



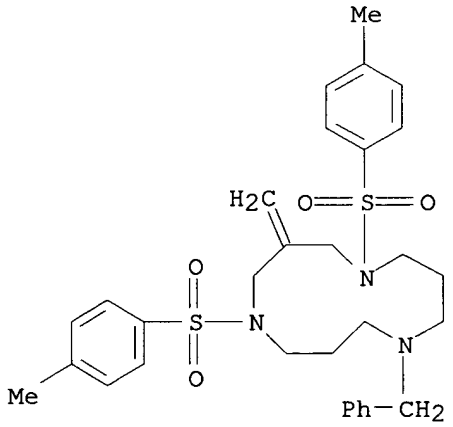
RN 182316-20-7 CAPLUS
CN 1,5,9-Triazacyclododecan-3-one, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



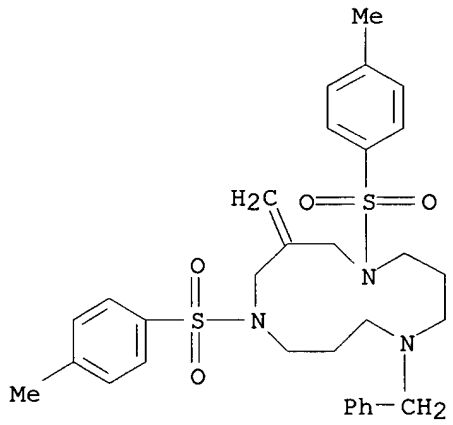
RN 182316-30-9 CAPLUS
CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 182316-44-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

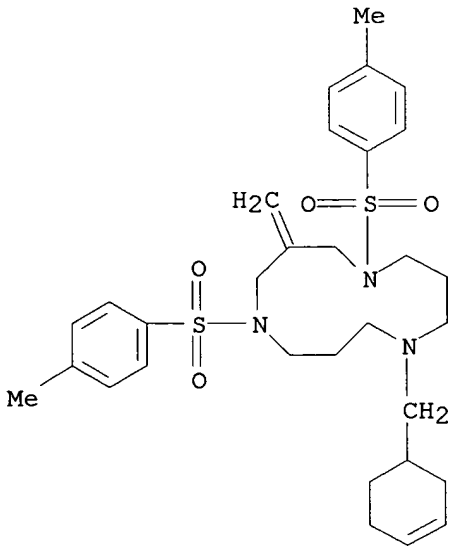


RN 392287-03-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

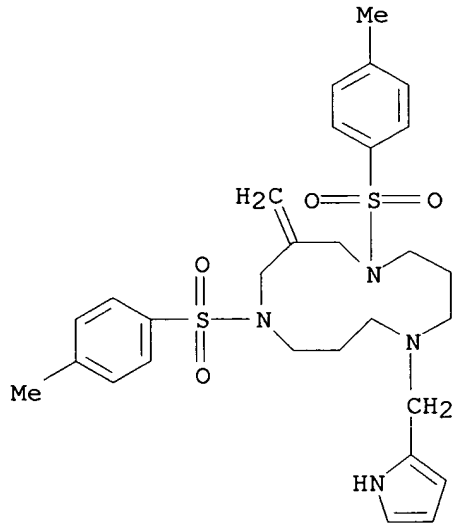


● HCl

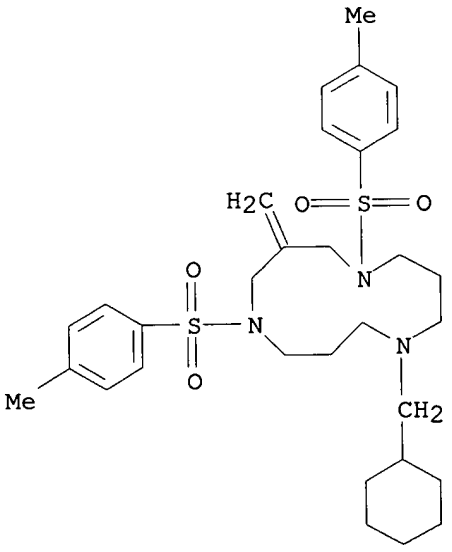
RN 471866-86-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(3-cyclohexen-1-ylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



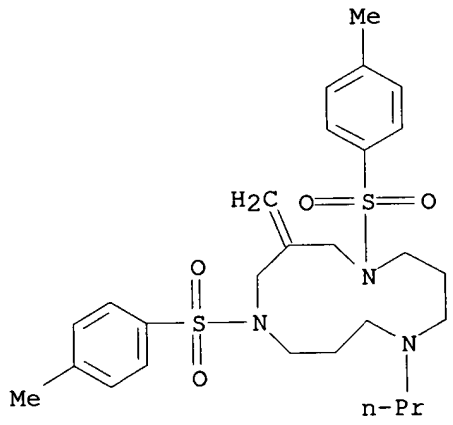
RN 471866-87-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(1H-pyrrol-2-ylmethyl)- (9CI) (CA INDEX NAME)



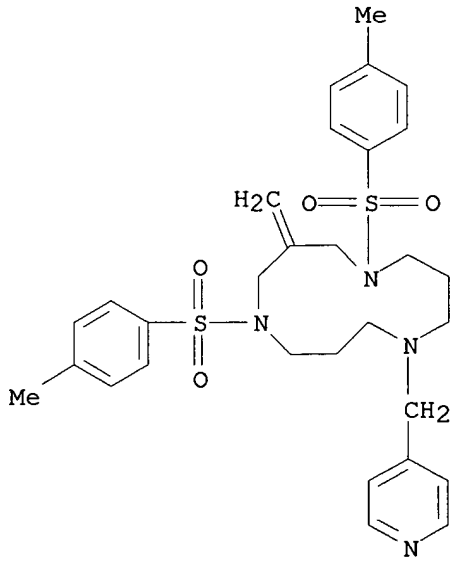
RN 471866-89-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(cyclohexylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



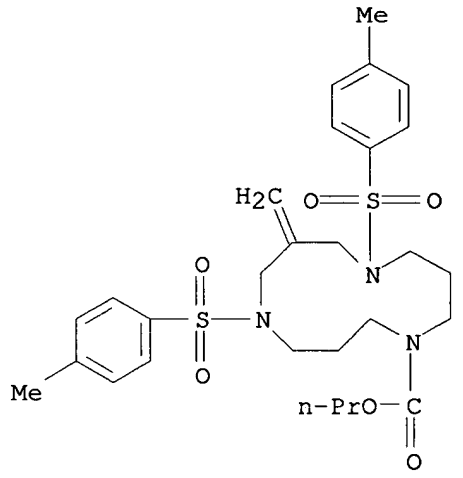
RN 471866-90-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-propyl- (9CI) (CA INDEX NAME)



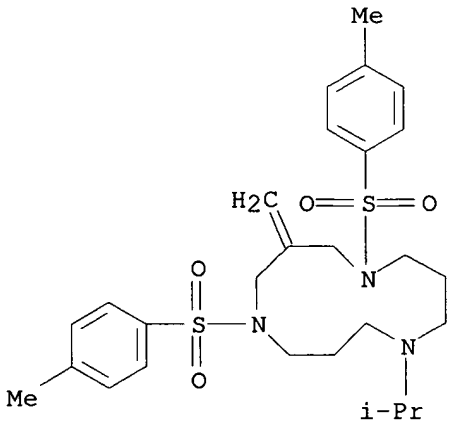
RN 471866-91-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



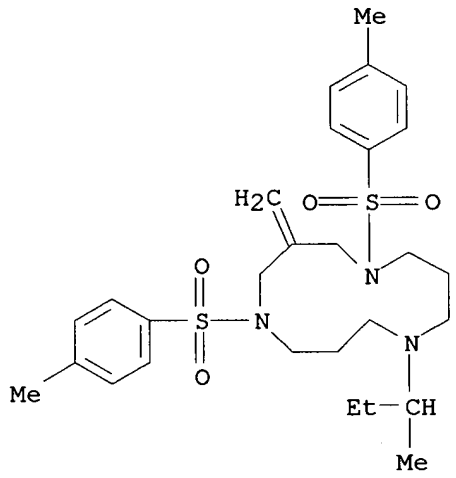
RN 471866-92-9 CAPLUS
CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, propyl ester (9CI) (CA INDEX NAME)



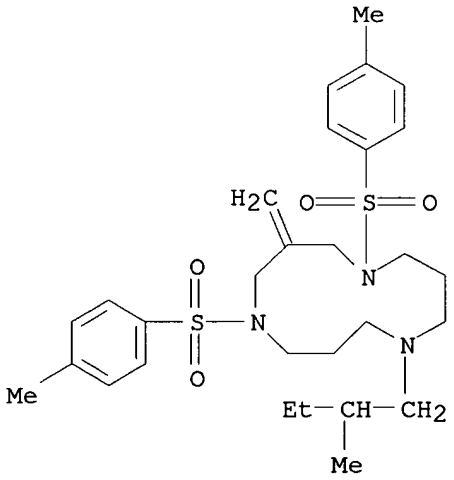
RN 471866-93-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-9-(1-methylethyl)-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



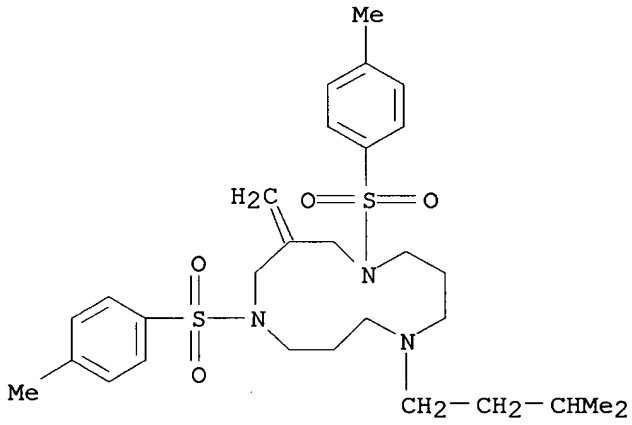
RN 471866-94-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(1-methylpropyl)- (9CI) (CA INDEX NAME)



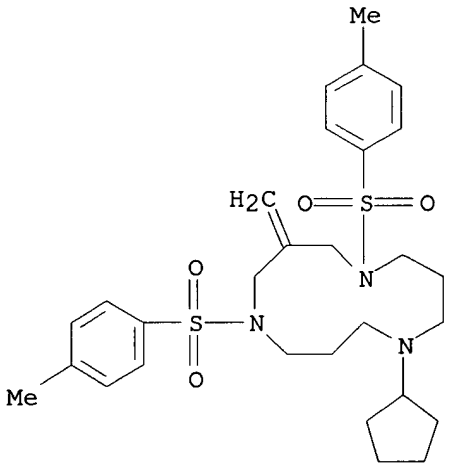
RN 471866-95-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(2-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



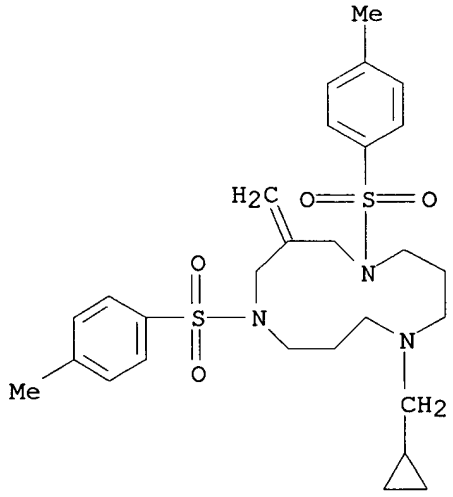
RN 471866-96-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(3-methylbutyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



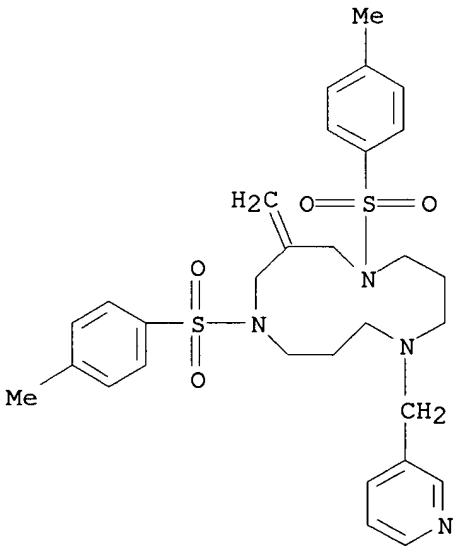
RN 471866-97-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-cyclopentyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



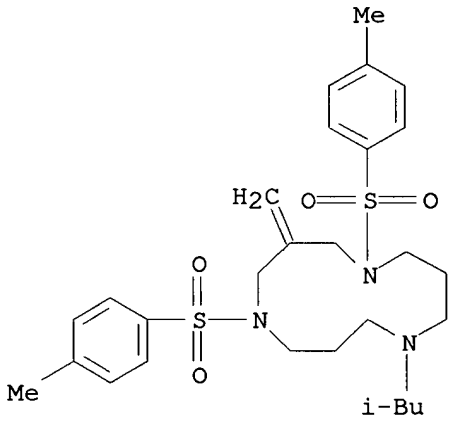
RN 471866-98-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(cyclopropylmethyl)-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 471866-99-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

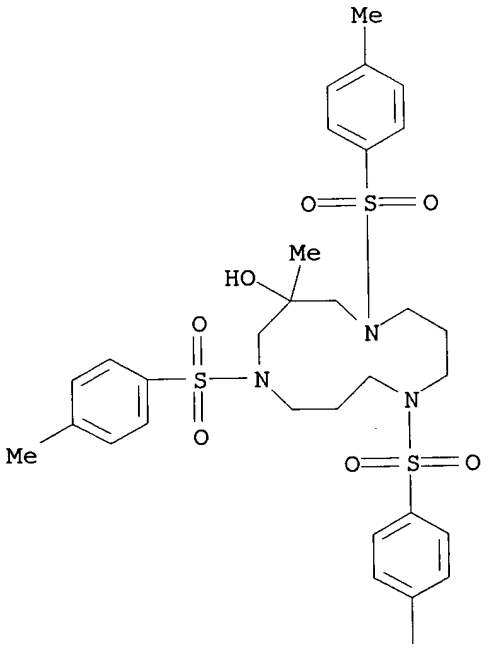


RN 471867-00-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-methylpropyl)- (9CI) (CA INDEX NAME)



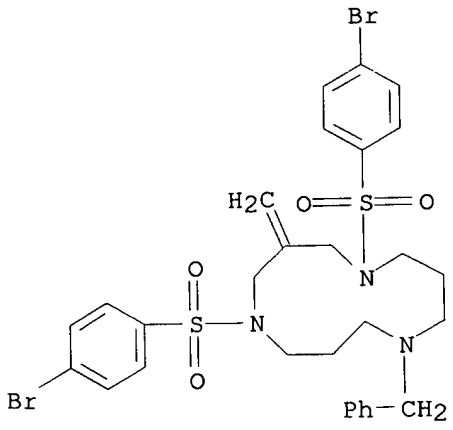
RN 471867-01-3 CAPLUS
CN 1,5,9-Triazacyclododecan-3-ol, 3-methyl-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



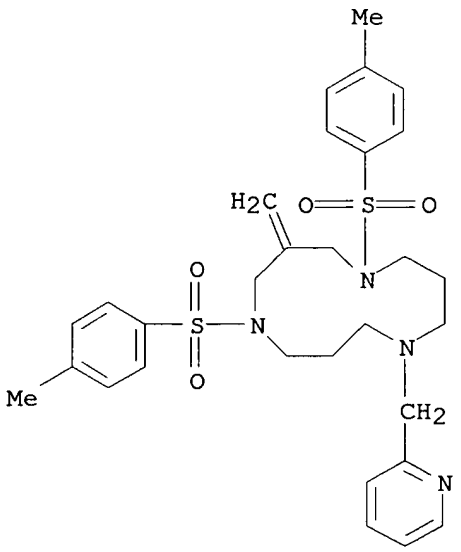
PAGE 2-A

RN 471867-02-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-bromophenyl)sulfonyl]-3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

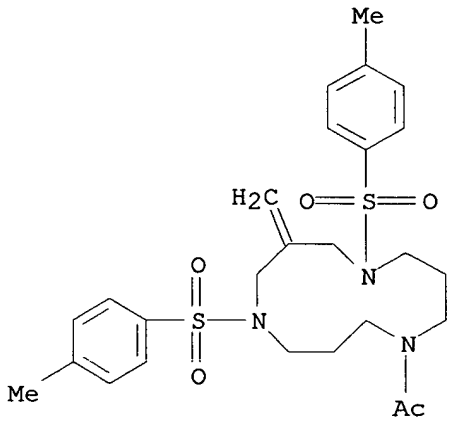


RN 471867-03-5 CAPLUS

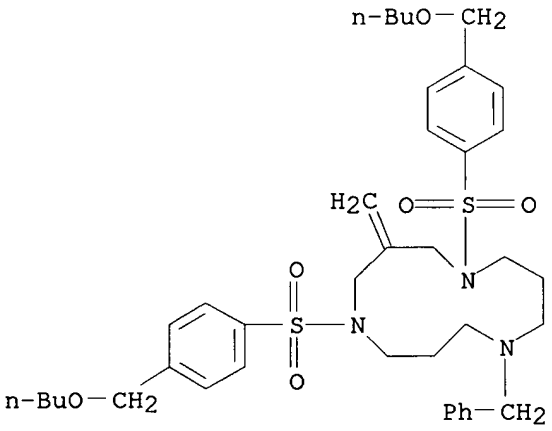
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



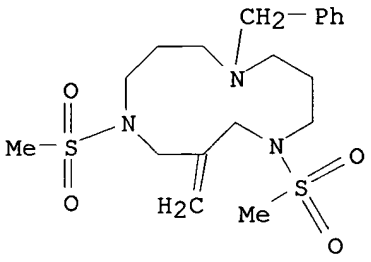
RN 471867-04-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-acetyl-3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



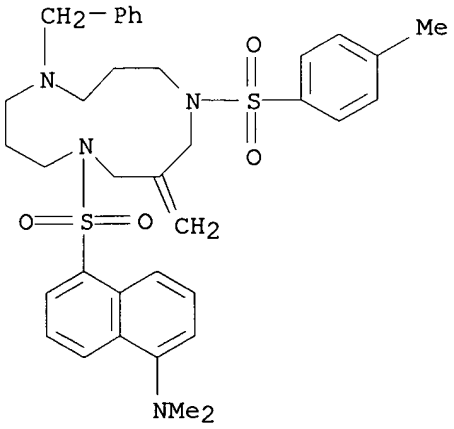
RN 471867-05-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[[4-(butoxymethyl)phenyl]sulfonyl]-3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



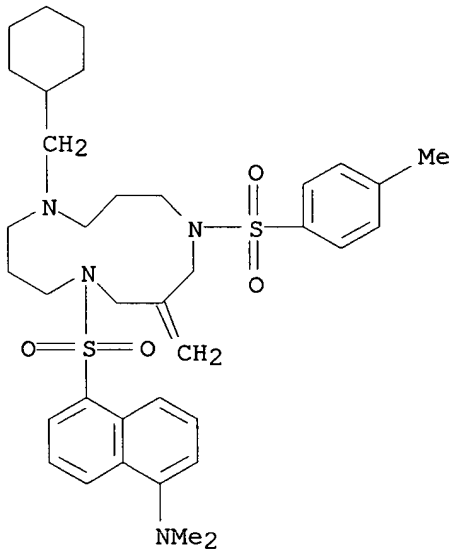
RN 471867-06-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis(methylsulfonyl)-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT 471866-79-2P 471866-80-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and biol. activity of naphthalenesulfonyl triazamacrocycles as immunoregulatory agents)
RN 471866-79-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 1-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]-3-methylene-5-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



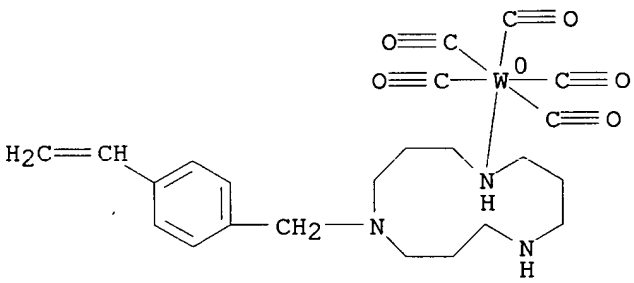
RN 471866-80-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 9-(cyclohexylmethyl)-1-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]-3-methylene-5-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



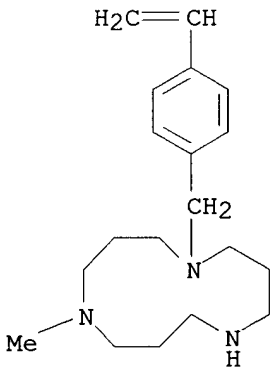
L20 ANSWER 15 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:359518 CAPLUS
DOCUMENT NUMBER: 137:194461
TITLE: Synthesis, characterisation and polymerization of vinylbenzene-substituted triazacyclododecanes and their transition metal complexes
AUTHOR(S): Long, Nicholas J.; Parker, David G.; Speyer, Paul R.; White, Andrew J. P.; Williams, David J.
CORPORATE SOURCE: Department of Chemistry, Imperial College of Science, Technology and Medicine, South Kensington, London, SW7 2AY, UK
SOURCE: Journal of the Chemical Society, Dalton Transactions (2002), (10), 2142-2150
CODEN: JCSDAA; ISSN: 1472-7773
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:194461

AB The synthesis of a range of methylated and nonmethylated triazacyclododecane derivs. featuring the unsym. incorporation of a 4-vinylbenzene side-arm is reported, along with the x-ray crystal structure of an amidinium salt precursor, and NMR characterization of these ligands. The free amine, 1-(4-vinylbenzyl)-1,5,9-triazacyclododecane (5), was reacted with transition metal centers and the coordination chemical is discussed, with structural anal. of an unusual triply-bridged (via one aqua and two chloride ligands) Ni(II) dimer and a mononuclear W(CO)5 complex. Co-polymerization studies on 5 and its metal complexes with varying percentages of styrene show the formation of low and high (via crosslinking) mol. weight polymers.

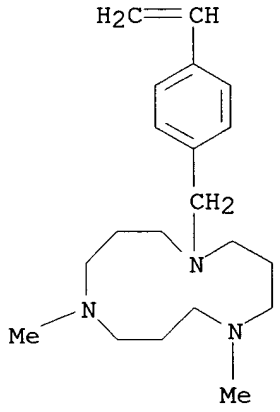
IT 448898-76-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure)
RN 448898-76-8 CAPLUS
CN Tungsten, pentacarbonyl[1-[(4-ethenylphenyl)methyl]-1,5,9-triazacyclododecane-κN5]-, (OC-6-22)- (9CI) (CA INDEX NAME)



IT 243670-33-9P, 1-Methyl-5-(4-vinylbenzyl)-1,5,9-triazacyclododecane
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation)
RN 243670-33-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 1-[(4-ethenylphenyl)methyl]-5-methyl- (9CI) (CA INDEX NAME)



IT 243670-34-0P, 5,9-Dimethyl-1-(4-vinylbenzyl)-1,5,9-triazacyclododecane
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 243670-34-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 1-[(4-ethenylphenyl)methyl]-5,9-dimethyl- (9CI) (CA INDEX NAME)



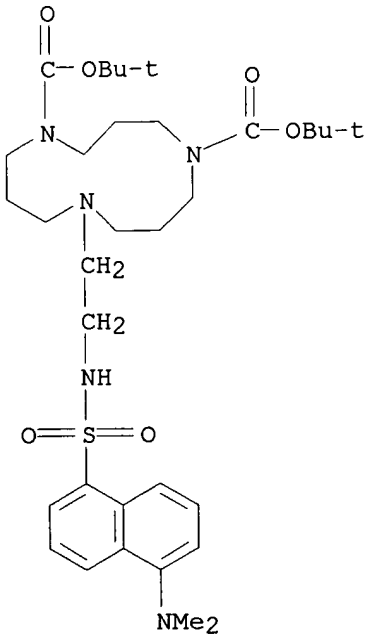
REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 16 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:271332 CAPLUS
DOCUMENT NUMBER: 137:118540
TITLE: Synthesis and characterization of the zinc(II)-fluorophore, 5-dimethylaminonaphthalene-1-sulfonic acid [2-(1,5,9-triazacyclododec-1-yl)ethyl]amide and its zinc(II) complex
AUTHOR(S): Koike, Tohru; Abe, Tomoko; Takahashi, Makoto; Ohtani, Kazuhiro; Kimura, Eiichi; Shiro, Motoo
CORPORATE SOURCE: Institute of Pharmaceutical Sciences, Faculty of Medicine, Hiroshima University, Minami-ku, Hiroshima, Japan
SOURCE: Journal of the Chemical Society, Dalton Transactions (2002), (8), 1764-1768
CODEN: JCSDAA; ISSN: 1472-7773
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:118540

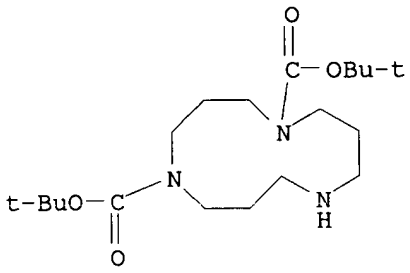
AB A new Zn(II)-fluorophore, 5-dimethylaminonaphthalene-1-sulfonic acid [2-(1,5,9-triazacyclododec-1-yl)ethyl]amide (HL) was synthesized and characterized. The spectrophotometric and potentiometric pH-titration study disclosed a 1:1 Zn(II) complexation with a stability constant, K(ZnL) of 101.3 (= [ZnL]aH+/[Zn2+][HL]) at 25° with I = 0.10 (NaCl) in aqueous solution, where L is the dansylamide deprotonated ligand. The fluorescence intensity of ZnL at 538 nm (excitation at 320 nm) is 5.2 times greater than that of the ligand (HL·H+ form) in aqueous solution at pH 7.8 and 25° with I = 0.10 (NaCl). The x-ray crystal anal. of the Zn(II) complex [ZnL(ClO4)·EtOH] showed a four-coordinate Zn(II) with three N atoms of the macrocyclic triamine and the dansylamide N- anion.

IT 443643-93-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)

RN 443643-93-4 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, 9-[2-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]ethyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



IT 174192-40-6, 1,5-Bis(tert-butoxycarbonyl)-1,5,9-triazacyclododecane
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of aminonaphthalenesulfonyltriazacyclododecylethyl amide)
RN 174192-40-6 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

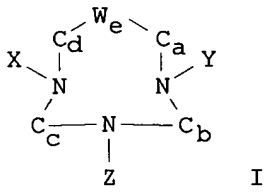


REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 17 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:84595 CAPLUS
DOCUMENT NUMBER: 136:129039
TITLE: Antiviral triaza compounds and compositions, and preparation thereof
INVENTOR(S): Bell, Thomas W.
PATENT ASSIGNEE(S): The Research Foundation of State University of New York, USA
SOURCE: U.S., 19 pp., Cont.-in-part of U.S. 5,663,161.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6342492	B1	20020129	US 1997-894491	19970807
US 5663161	A	19970902	US 1995-392550	19950217
WO 9625167	A1	19960822	WO 1996-US2132	19960216
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 2002019423	A1	20020214	US 2001-769021	20010125
PRIORITY APPLN. INFO.:			US 1995-392550	A2 19950217
			WO 1996-US2132	W 19960216
			US 1997-894491	A1 19970807

OTHER SOURCE(S): MARPAT 136:129039
GI



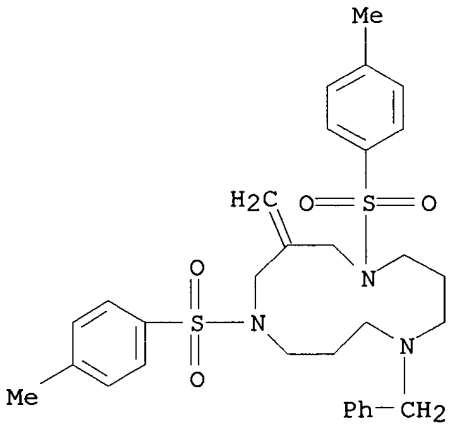
I

AB Synthetic triaza compds. I (W = bridge carbon with polar or nonpolar side group; X, Y = aromatic group, alkyl group, sulfonyl group, , carbonyl group; Z = X, Y, H, fused aryl; a, d, e = 0-10, b, c = 1-10) are disclosed which can be used in antiviral pharmaceutical compns. Preparation of e.g. 9-benzyl-3-methylene-1,5-ditosyl-1,5,9-triazacyclododecane is described. Synthesis of open-chain analogs is also described.

IT 182316-44-5P
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(antiviral triaza compds., compns., and preparation)

RN 182316-44-5 CAPLUS

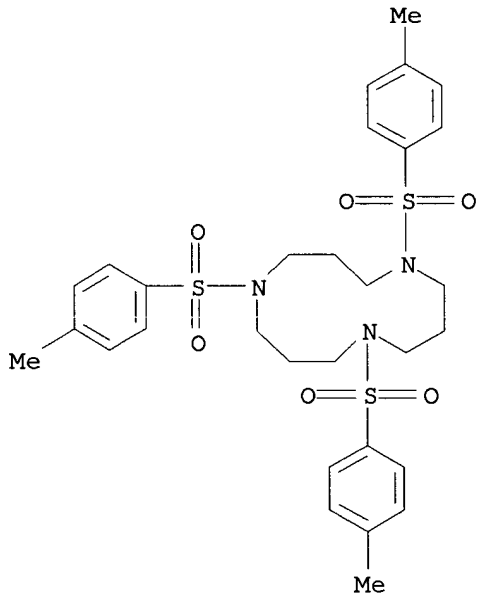
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT 35980-67-7P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(antiviral triaza compds., compns., and preparation)

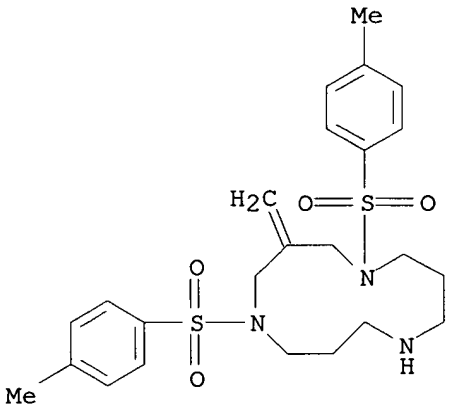
RN 35980-67-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



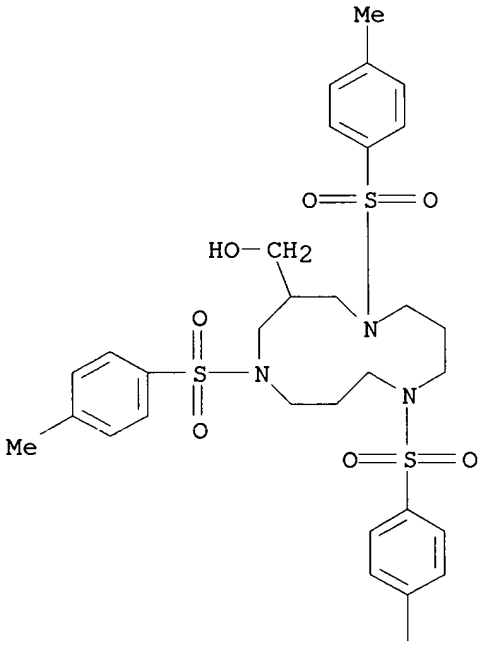
IT 182316-06-9 182316-17-2
RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(antiviral triaza compds., compns., and preparation)

RN 182316-06-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 182316-17-2 CAPLUS
CN 1,5,9-Triazacyclododecane-3-methanol, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

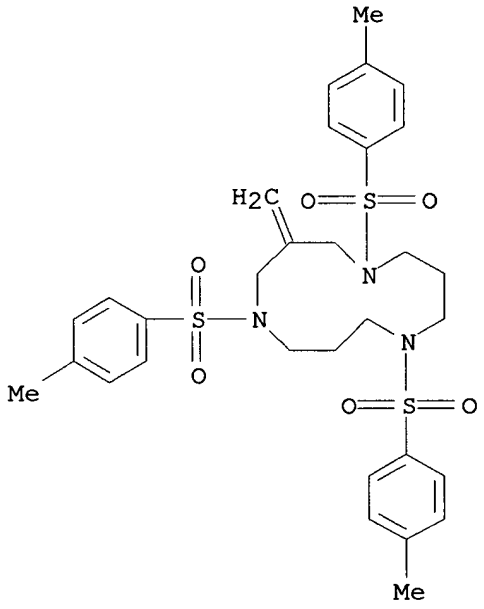


PAGE 2-A

Me

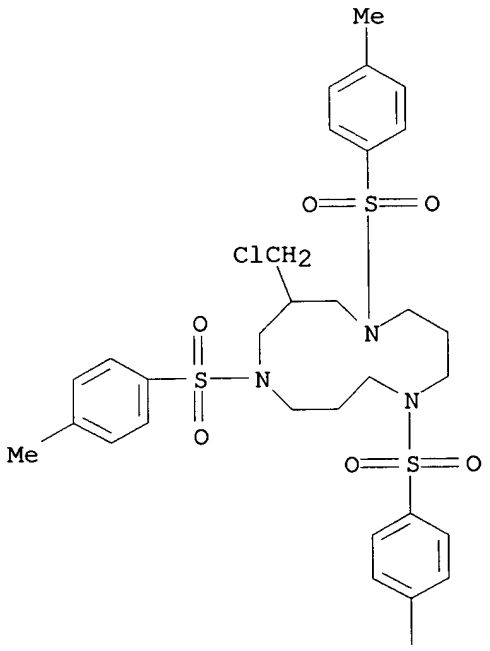
IT 182316-15-0P 182316-19-4P 182316-22-9P
182316-30-9P 182316-34-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antiviral triaza compds., compns., and preparation)

RN 182316-15-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



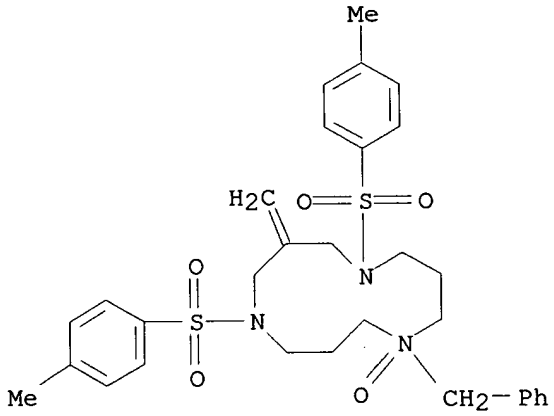
RN 182316-19-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



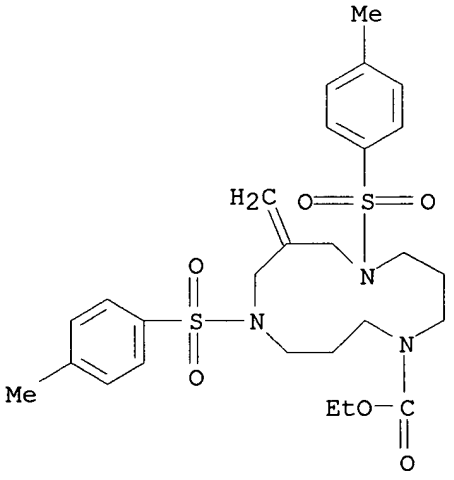
PAGE 2-A

RN 182316-22-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)-, 9-oxide (9CI) (CA INDEX NAME)

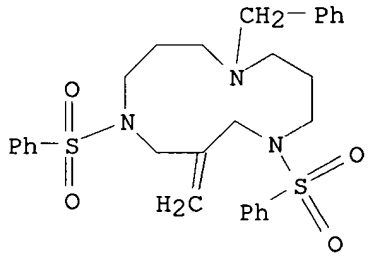


RN 182316-30-9 CAPLUS

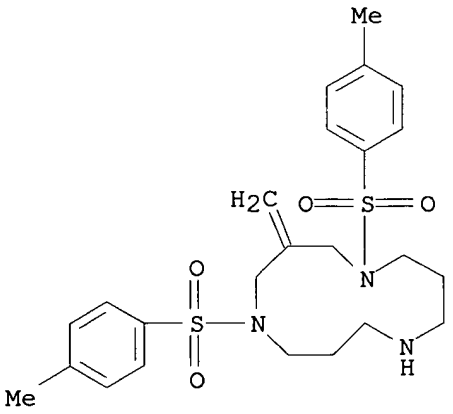
CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)



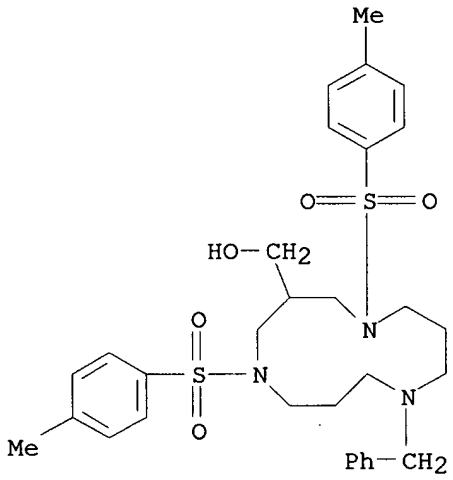
RN 182316-34-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-9-(phenylmethyl)-1,5-bis(phenylsulfonyl)- (9CI) (CA INDEX NAME)



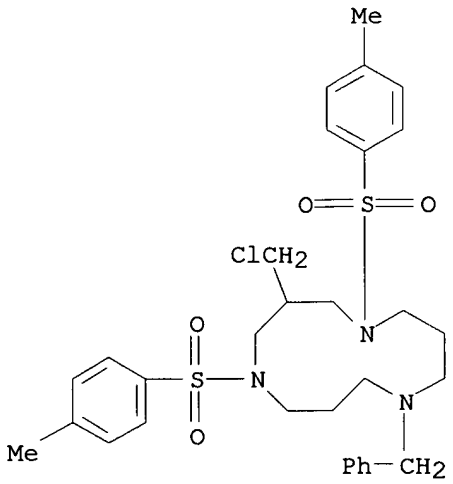
IT 182316-06-9D, derivs. 182316-08-1 182316-10-5
182316-12-7 182316-20-7 182316-21-8
182316-25-2 182316-27-4 182316-27-4D, acylated
392287-02-4 392287-03-5 392287-04-6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antiviral triaza compds., compns., and preparation)
RN 182316-06-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



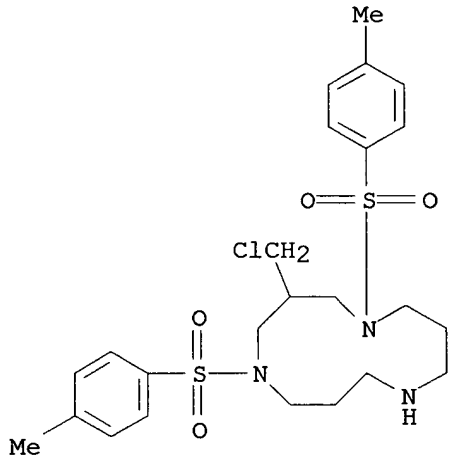
RN 182316-08-1 CAPLUS
CN 1,5,9-Triazacyclododecane-3-methanol, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



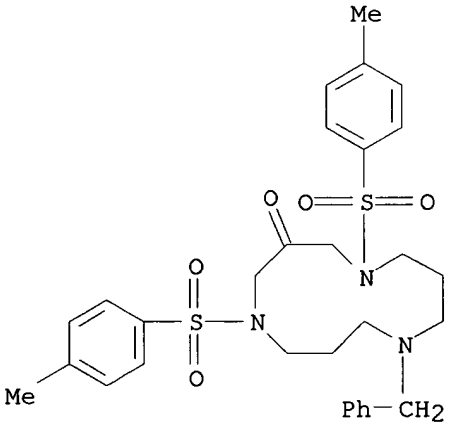
RN 182316-10-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



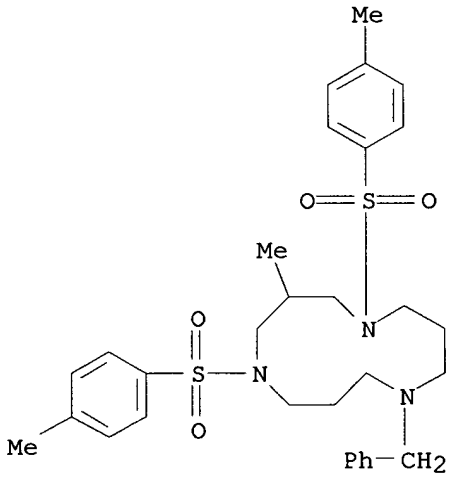
RN 182316-12-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



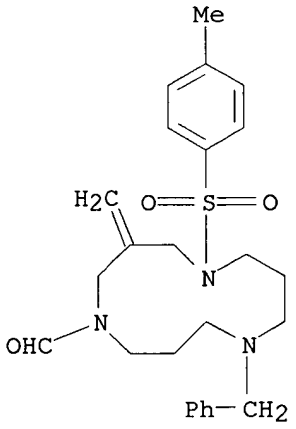
RN 182316-20-7 CAPLUS
CN 1,5,9-Triazacyclododecan-3-one, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



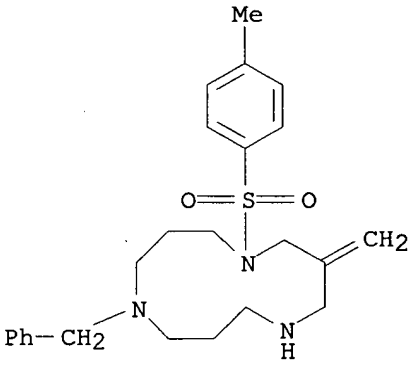
RN 182316-21-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methyl-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



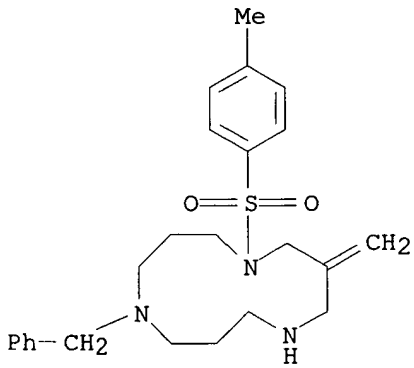
RN 182316-25-2 CAPLUS
CN 1,5,9-Triazacyclododecane-1-carboxaldehyde, 3-methylene-5-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



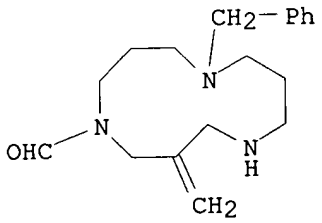
RN 182316-27-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



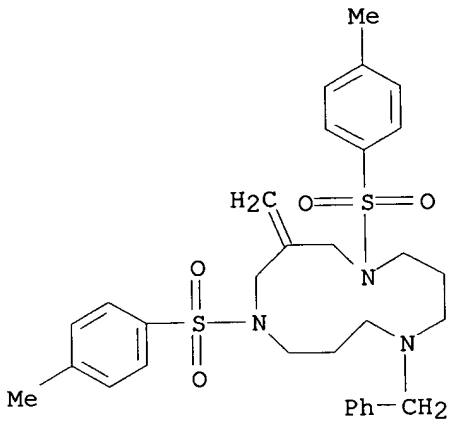
RN 182316-27-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 392287-02-4 CAPLUS
CN 1,5,9-Triazacyclododecane-1-carboxaldehyde, 3-methylene-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

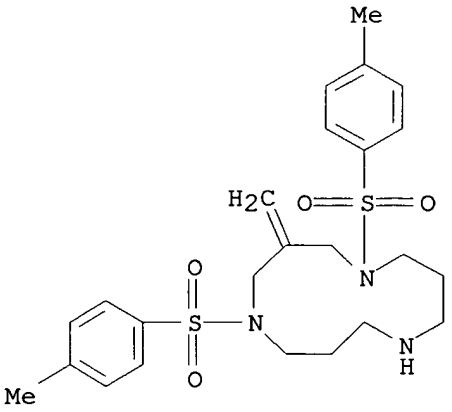


RN 392287-03-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



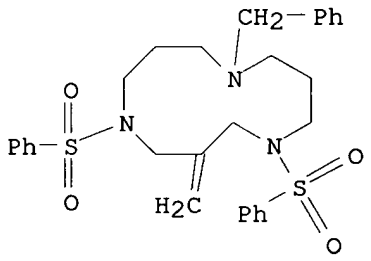
● HCl

RN 392287-04-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

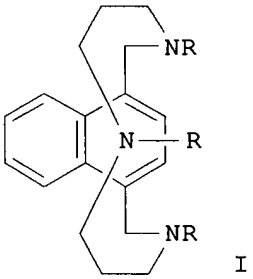
IT 182316-50-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(antiviral triaza compds., compns., and preparation)
RN 182316-50-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-9-(phenylmethyl)-1,5-bis(phenylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)



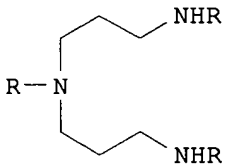
● HCl

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 18 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:218085 CAPLUS
DOCUMENT NUMBER: 135:5605
TITLE: Synthesis of Polyazamacrocyclic Compounds via Modified Richman-Atkins Cyclization of β-Trimethylsilylethanesulfonamides
AUTHOR(S): Hoye, Rebecca C.; Richman, Jack E.; Dantas, Gautam A.; Lightbourne, Marissa F.; Shinneman, L. Scott
CORPORATE SOURCE: Department of Chemistry, Macalester College, St. Paul, MN, 55105, USA
SOURCE: Journal of Organic Chemistry (2001), 66(8), 2722-2725
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:5605
GI



I

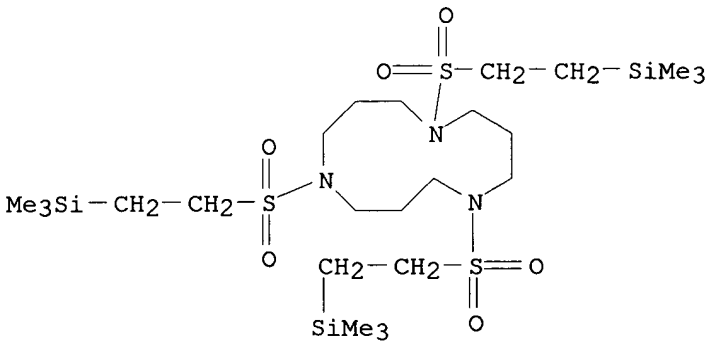


II

AB The use of β-trimethylsilylethanesulfonamides (SES-sulfonamides) for the preparation of polyazamacrocyclic compds. is described. This expands existing Richman-Atkins sulfonamide macrocyclization methodol., and it successfully enables preparation of labile polyaza[n](1,4)naphthalenophanes and polyaza[n](9,10)anthracenophanes, not previously available in appreciable quantities. Thus, triazanaphthalenecyclophane I (R = Me3SiCH2CH2SO2) was prepared from 1,4-bis(bromomethyl)naphthalene and the trimethylethanesulfonamide II.

IT 340970-56-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of azacyclophanes via Richman-Atkins cyclization of trimethylsilylethanesulfonamides with ditosylates or bis(bromomethyl) compds.)

RN 340970-56-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris[[2-(trimethylsilyl)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

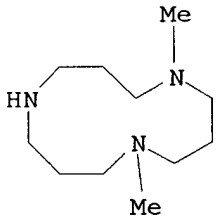


REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

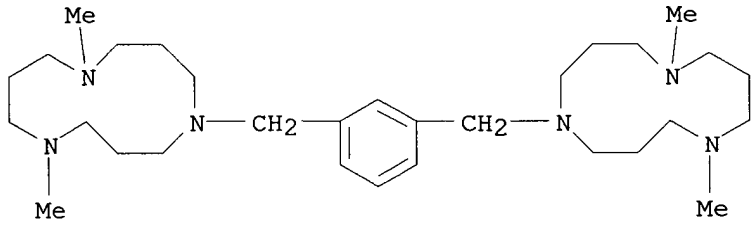
L30 ANSWER 19 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:107172 CAPLUS
DOCUMENT NUMBER: 134:277328
TITLE: Remarkable cooperative action of two zinc centers in the hydrolysis of plasmid DNA
AUTHOR(S): Aka, F. Nihan; Akkaya, Mahinur S.; Akkaya, Engin U.
CORPORATE SOURCE: Department of Chemistry, Middle East Technical University, Ankara, TR-06531, Turk.
SOURCE: Journal of Molecular Catalysis A: Chemical (2001), 165(1-2), 291-294
CODEN: JMCCF2; ISSN: 1381-1169
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A novel binuclear zinc complex has been synthesized. The complex is highly efficient in the hydrolysis of plasmid DNA at pH 7.5. Furthermore, a comparison to a mononuclear complex reveals a high level of cooperativity between the two metal ion centers.

IT 139258-69-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(preparation and DNA hydrolytic activity of binuclear zinc complex)
RN 139258-69-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-dimethyl- (9CI) (CA INDEX NAME)



IT 333784-11-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and DNA hydrolytic activity of binuclear zinc complex)
RN 333784-11-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,1'-[1,3-phenylenebis(methylene)]bis[5,9-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

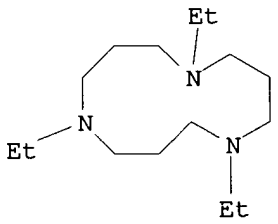
L80 ANSWER 20 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:69121 CAPLUS
DOCUMENT NUMBER: 134:131928
TITLE: Epoxidation catalysts and production method of epoxidized compounds of olefins therewith
INVENTOR(S): Sakamoto, Takaki; Park, Chong Jin
PATENT ASSIGNEE(S): Kawamura Institute of Chemical Research, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001025665	A2	20010130	JP 1999-202402	19990716
PRIORITY APPLN. INFO.:			JP 1999-202402	19990716

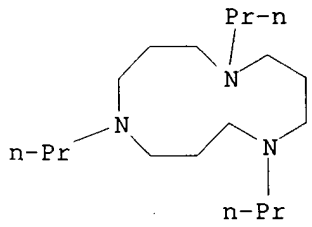
AB Title catalysts comprise (1) methyltrioxorhenium (CH3ReO3) and (2) cyclic triamines selected from 1,4,7-trimethyl-1,4,7-triazacyclononane, 1,4,7-triethyl-1,4,7-triazacyclononane, 1,4,7-tripropyl-1,4,7-triazacyclononane, 1,5,9-trimethyl-1,5,9-triazacyclododecane, 1,5,9-triethyl-1,5,9-triazacyclododecane, and 1,5,9-tripropyl-1,5,9-triazacyclododecane on supports selected from alumina, silica gel, and florisil. Thus, 0.246 g cyclohexane was reacted with 0.68 g 30% H2O2 in water in the presence of a catalyst comprising methyltrioxorhenium 250, 1,4,7-trimethyl-1,4,7-triazacyclononane 171, and silica gel 500 mg to give a cyclohexane oxide with conversion rate and selectivity 100%.

IT 321861-36-3 321861-37-4
RL: CAT (Catalyst use); USES (Uses)
(epoxidn. catalysts for preparation of epoxy compds. from olefins)

RN 321861-36-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-triethyl- (9CI) (CA INDEX NAME)



RN 321861-37-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tripropyl- (9CI) (CA INDEX NAME)

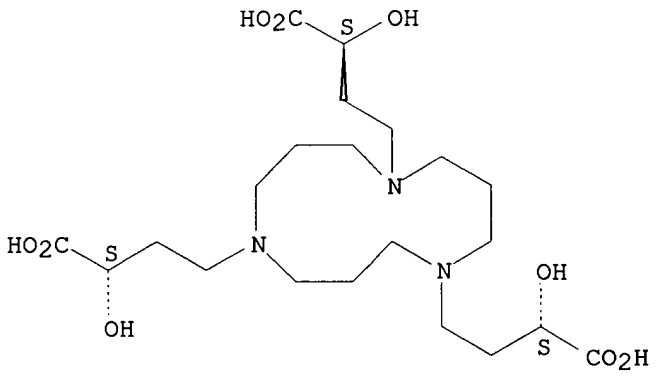


L80 ANSWER 21 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:695769 CAPLUS
DOCUMENT NUMBER: 133:355853
TITLE: Mn2+, Co2+, Cu2+ and Zn2+ complexes with two macrocyclic ligands bearing L-lactate-like functions: potentiometric studies and evaluation of superoxide-scavenging properties of the Mn2+ complex
AUTHOR(S): Delagrange, Samuel; Delgado, Rita; Nepveu, Francoise
CORPORATE SOURCE: Laboratoire Pharmacophores Redox, Phytochimie et Radiobiologie, Universite Paul Sabatier 35, Toulouse, 31062, Fr.
SOURCE: Journal of Inorganic Biochemistry (2000), 81(1-2), 65-71
CODEN: JIBIDJ; ISSN: 0162-0134
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Some aerobic organisms devoid of SOD use Mn2+ chelates to scavenge the O2- radical. Since the Mn2+-bis(lactato)diaquo complex is known as having a high SOD-like activity, the authors prepared manganese(II) complexes with triazamacrocyclic ligands bearing L-lactate-like functions to obtain model compds. able to disproportionate the superoxide radical. Thus, two macrocyclic ligands, N,N',N''-tris[2(S)-hydroxybutyric acid]-1,4,7-triazacyclononane, L1, and N,N',N''-tris[2(S)-hydroxybutyric acid]-1,5,9-triazacyclododecane, L2, were prepared (prior work) and their capacity to retain the Mn2+ ion in aqueous solution was determined from potentiometric expts. The chelating properties in aqueous solution of each ligand towards Co2+, Cu2+ and Zn2+ ions were also determined L1 forms complexes with Mn2+, Co2+, Cu2+ and Zn2+ ions with stability consts. of 8.33(5), 15.78(5), 17.65(3) and 14.32(1), resp. L2 forms complexes with Cu2+ and Zn2+ ions with stability consts. of 10.67(1) and 6.98(3), resp. But the consts. related to the Mn2+ and Co2+ complexes were too low to be determined by the method used. The stability consts. values calculated for L2 complexes are significantly lower than those for the corresponding complexes of L1. Addnl. spectroscopic measurements were carried out on the Mn2+-L1 system. The electronic spectrum of this system showed a pH-dependence that may be consistent with the formation of hydroxo-species as the ESR spectra recorded at 120 K did not show oxidation of the Mn2+ ion in the pH range studied. The superoxide-scavenging activity of the manganese(II)-L1 complex was investigated using the cytochrome c assay. The Mn2+-L1 system showed an IC50 value of 1.7 μM which indicates that it appears as a potent SOD mimic.

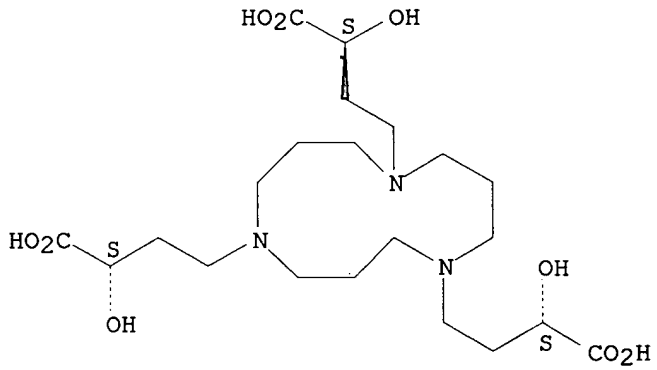
IT 241486-68-0
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(protonation consts. and complexation with transition metals)
RN 241486-68-0 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tributanoic acid, α,α',α''-trihydroxy-, (αS,α'S,α''S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 241486-68-0D, copper and zinc complexes
RL: CAT (Catalyst use); FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative); USES (Uses)
(stability consts.)
RN 241486-68-0 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tributanoic acid, α,α',α''-trihydroxy-, (αS,α'S,α''S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



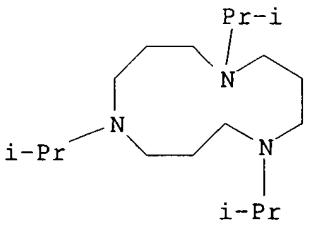
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 22 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:554692 CAPLUS
DOCUMENT NUMBER: 133:275527
TITLE: Ligand Macrocycle Structural Effects on Copper-Dioxygen Reactivity
AUTHOR(S): Lam, Bernice M. T.; Halfen, Jason A.; Young, Victor G., Jr.; Hagadorn, John R.; Holland, Patrick L.; Lledos, Agusti; Cucurull-Sanchez, Lourdes; Novoa, Juan J.; Alvarez, Santiago; Tolman, William B.
CORPORATE SOURCE: Department of Chemistry and Center for Metals in Biocatalysis, University of Minnesota, Minneapolis, MN, 55455, USA
SOURCE: Inorganic Chemistry (2000), 39(18), 4059-4072
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB With the goal of understanding how the nature of the tridentate macrocyclic supporting ligand influences the relative stability of isomeric μ-η2:η2-peroxo- and bis(μ-oxo)dicopper complexes, a comparative study was undertaken of the O2 reactivity of Cu(I) compds. supported by the 10- and 12-membered macrocycles, 1,4,7-R3-1,4,7-triazacyclodecane (R3TACD; R = Me, Bn, iPr) and 1,5,9-triisopropyl-1,5,9-triazacyclododecane (iPr3TACDD). While the 3-coordinate complex [(iPr3TACDD)Cu]SbF6 was unreactive with O2, oxygenation of [(R3TACD)Cu(MeCN)]X (R = Me or Bn; X = ClO4- or SbF6-) at -80° yielded bis(μ-oxo) species [(R3TACD)2Cu2(μ-O)2]X2 as revealed by UV-visible and resonance Raman spectroscopy. Interestingly, unlike the previously reported system supported by 1,4,7-triisopropyl-1,4,7-triazacyclononane (iPr3TACN), which yielded interconverting mixts. of peroxo and bis(μ-oxo) compds. (Cahoy, J.; Holland, P. L.; Tolman, W. B. Inorg. Chemical 1999, 38, 2161), low-temperature oxygenation of [(iPr3TACD)Cu(MeCN)]SbF6 in a variety of solvents cleanly yielded a μ-η2:η2-peroxo product, with no trace of the bis(μ-oxo) isomer. The peroxo complex was characterized by UV-visible and resonance Raman spectroscopy, as well as an x-ray crystal structure (albeit of marginal quality due to disorder problems). Intramol. attack at the α C-H bonds of the substituents was indicated as the primary decomposition pathway of the oxygenated compds. through examination of the decay kinetics and the reaction products, which included bis(μ-hydroxo)- and μ-carbonato-dicopper complexes that were characterized by x-ray diffraction. A rationale for the varying results of the oxygenation reactions was provided by anal. of (a) the x-ray crystal structures and electrochem. behavior of the Cu(I) precursors and (b) the results of theor. calcns. of the complete oxygenated complexes, including all ligand atoms, using combined quantum chemical/mol. mechanics (integrated MO mol. mechanics, IMOMM) methods. The size of the ligand substituents is a key factor in controlling the relative stabilities of the peroxo and bis(μ-oxo) forms, and the nature of this influence was shown by both theory and experiment to depend on the ligand macrocycle ring size.

IT 296761-76-7P, 1,5,9-Triisopropyl-1,5,9-triazacyclododecane
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, complexation with copper(I), and influence of ring size on copper-dioxygen reactivity)
RN 296761-76-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris(1-methylethyl)- (9CI) (CA INDEX

NAME)



REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 23 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

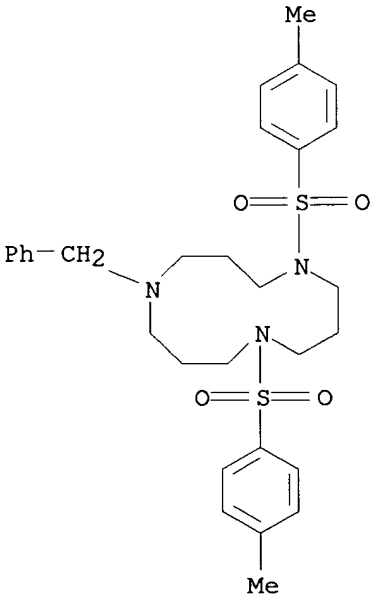
ACCESSION NUMBER: 2000:165352 CAPLUS
DOCUMENT NUMBER: 132:321849
TITLE: Multi-layer macromonocyclic polyamines. I. Molecular design and synthesis of component monocyclic precursors
AUTHOR(S): Iwata, Masaaki
CORPORATE SOURCE: Biopolymer Phys. Lab., The Institute of Physical and Chemical Research (RIKEN), Wako, Saitama, 351-0198, Japan
SOURCE: Bulletin of the Chemical Society of Japan (2000), 73(3), 693-704
CODEN: BCSJA8; ISSN: 0009-2673
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:321849
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

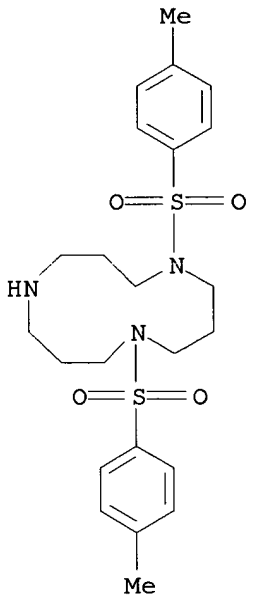
AB Multi-layer macromonocyclic polyamines, which might be appropriate polymorphismic mol. scaffolds as host-mols. in ionic or mol. interaction with small or large guest ions or mols, have been designed. In polymorphismic mols., several macromonocyclic polyamines with the same and/or different ring sizes and nitrogen contents are connected to each other by alkylene spacers with various length of chain. Actual target mols. were characterized by possessing methylene chain arrays of natural polyamines. Fourteen component macromonocycles of various sizes, e.g. 12- to 34-membered rings containing three to eight nitrogen atoms, were prepared from simple starting materials as essential building blocks required for construction of multi-layer mols. The synthetic method was very efficient. In a final step, the N-protecting benzyl group was successfully removed by hydrogenation on 10%-Pd/C under 4 kg cm-2 H2 to give the cyclic amine precursors, e.g. I and II, which could be internal and terminal components in the architecture of the multi-layer mols. The structures of synthesized compds. were characterized and confirmed by elemental anal., 1H-NMR, and SIMS and FAB(+) mass spectrometry.

IT 164913-15-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of macromonocyclic polyamines and mol. design of multi-layer macromonocyclic polyamines)

RN 164913-15-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT 164913-31-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of macromonocyclic polyamines and mol. design of multi-layer macromonocyclic polyamines)
RN 164913-31-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



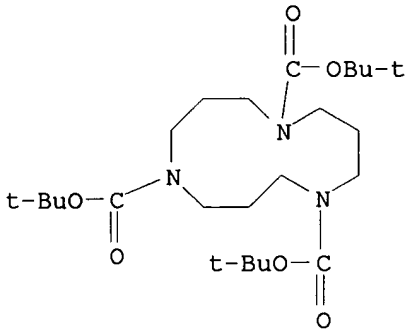
REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L80 ANSWER 24 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:119093 CAPLUS
DOCUMENT NUMBER: 132:216106
TITLE: The first dicopper(II) complex of a new bis(1,5,9-triazacyclododecane) ligand: synthesis, crystal structure and magnetic coupling of the complex
AUTHOR(S): Bu, Xian-He; Lu, Shou-Liang; Zhang, Ruo-Hua; Liao, Dai-Zheng; Aoki, Shin; Clifford, Thomas; Kimura, Eiichi
CORPORATE SOURCE: Department of Chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China
SOURCE: Inorganica Chimica Acta (2000), 298(1), 50-56
CODEN: ICHAA3; ISSN: 0020-1693
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new binucleating macrocyclic polyamine ligand based on 1,5,9-triazacyclododecane ([12]aneN3), 2,6-bis(1,5,9-triazacyclododecan-9-ylmethyl)benzoic acid (HL), was synthesized from a selectively Boc protected [12]aneN3 precursor and 2,6-bis(bromomethyl) benzoate. L can form a stable binuclear complex with Cu(II) in aqueous solution, [Cu2L(N3)2]ClO4, which was characterized by x-ray crystallog. (monoclinic, space group Cc, R = 0.069). The intramol. binuclear Cu(II) centers are bridged by a μ-carboxyl group on L and separated by 5.947 Å. Both of the Cu(II) centers are coordinated by three amine nitrogens of [12]aneN3 subunit and one oxygen of the carboxyl group, as well as one azide anion, and each Cu(II) center is in a distorted state intermediate between a square-pyramid and trigonal-bipyramid environment. This is the 1st binuclear Cu(II) complex formed with a bis([12]aneN3) ligand. Variable temperature magnetic susceptibility studies indicate that there exists intramol. antiferromagnetic coupling (-2J = 71.4 cm-1) between the two unpaired electrons of the two Cu(II) ions in the complex.

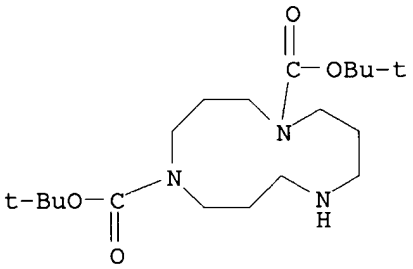
IT 260433-36-1P, 1,5,9-Tris(N-tert-butoxycarbonyl)-1,5,9-triazacyclododecane
RL: BYP (Byproduct); PREP (Preparation)
(byproduct in preparation of copper(II) bis(triazacyclododecanylmethyl)benzoato azido dinuclear complex)

RN 260433-36-1 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxylic acid, tris(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

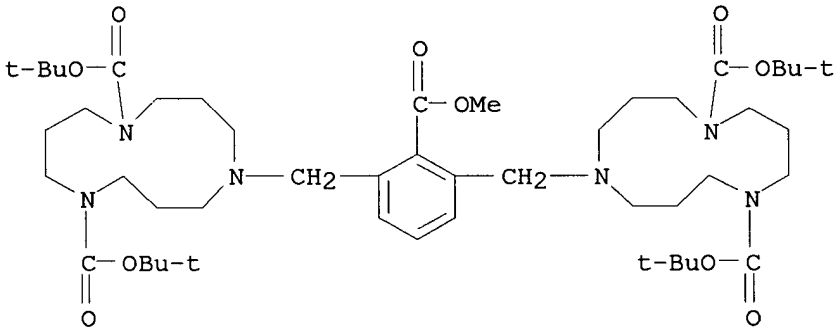


IT 174192-40-6P, 1,5-Bis(N-tert-butoxycarbonyl)-1,5,9-triazacyclododecane 260433-33-8P, Methyl 2,6-bis(1,5-bis(N-tert-butoxycarbonyl)-1,5,9-triazacyclododecan-9-ylmethyl)benzoate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of copper(II) bis(triazacyclododecanylmethyl)benzoato azido dinuclear complex)

RN 174192-40-6 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 260433-33-8 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, 9,9'-[[2-(methoxycarbonyl)-1,3-phenylene]bis(methylene)]bis-, tetrakis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

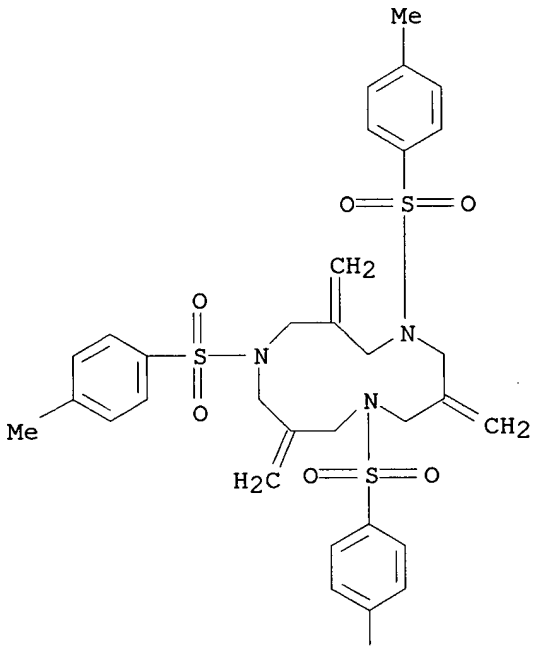
L80 ANSWER 25 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:777516 CAPLUS
DOCUMENT NUMBER: 132:137370
TITLE: Application of matrix-assisted laser desorption/ionization time-of-flight mass spectrometry to the structure determination of medium and large macrocycles formed by palladium(0)-catalyzed allylation of arenesulfonamides, sulfamide, and cyanamide
AUTHOR(S): Cerezo, Silvia; Cortes, Jordi; Galvan, David; Lopez-Romero, Juan-Manuel; Moreno-Manas, Marcial; Pleixats, Roser; Aviles, Francesc X.; Canals, Francesc; Roglans, Anna
CORPORATE SOURCE: Department of Chemistry, Universitat Autonoma de Barcelona, Barcelona, 08193, Spain
SOURCE: Rapid Communications in Mass Spectrometry (1999), 13(23), 2359-2365
CODEN: RCMSEF; ISSN: 0951-4198
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry allowed the direct determination of the extent of macrocyclic and linear oligomer formation in the palladium(0)-catalyzed allylation of highly acidic and non-nucleophilic arenesulfonamides, sulfamide, and cyanamide. Palladium-containing 15-membered-ring macrocyclic compds. gave unusual [M - H]+ ions besides [M + Na]+ and [M + K]+ adducts.

IT 130927-35-4 219839-43-7 219839-47-1
219839-49-3
RL: PRP (Properties)
(structure determination by MALDI-TOF mass spectrometry of cyclic compds. formed by palladium(0)-catalyzed allylation of arenesulfonamides, sulfamide, and cyanamide)

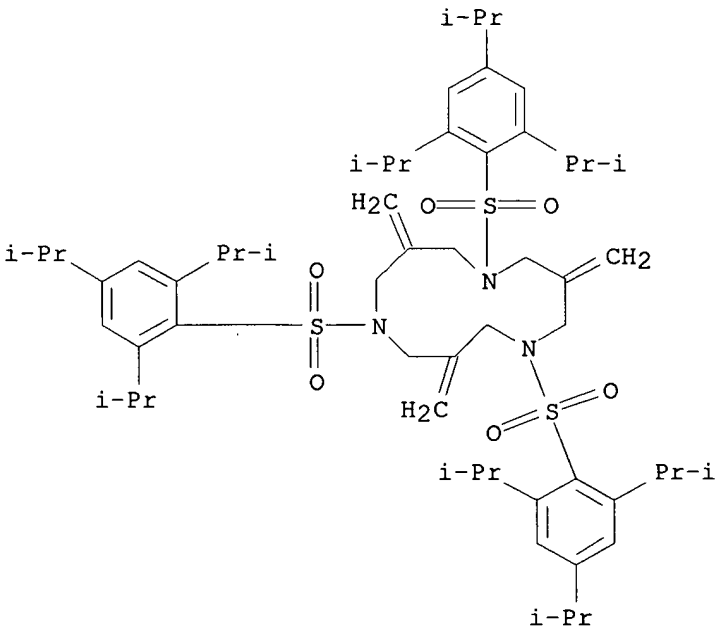
RN 130927-35-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

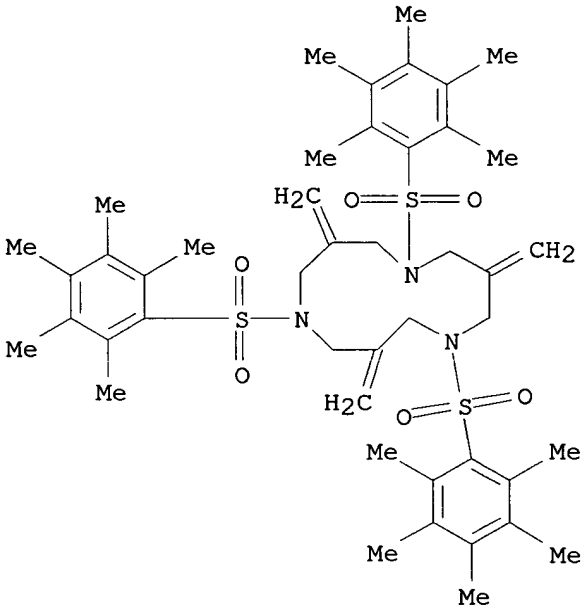


PAGE 2-A

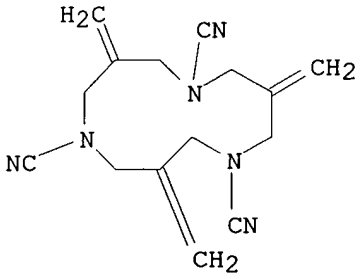
RN 219839-43-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[[2,4,6-tris(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



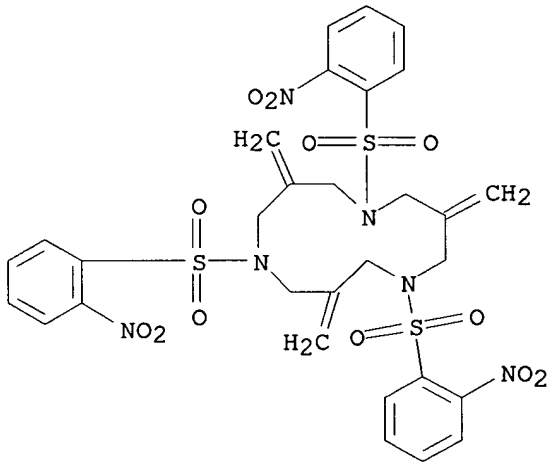
RN 219839-47-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[(pentamethylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 219839-49-3 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarbonitrile, 3,7,11-tris(methylene)- (9CI) (CA INDEX NAME)



IT 256498-09-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(structure determination by MALDI-TOF mass spectrometry of cyclic compds. formed by palladium(0)-catalyzed allylation of arenesulfonamides, sulfamide, and cyanamide)
RN 256498-09-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[(2-nitrophenyl)sulfonyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

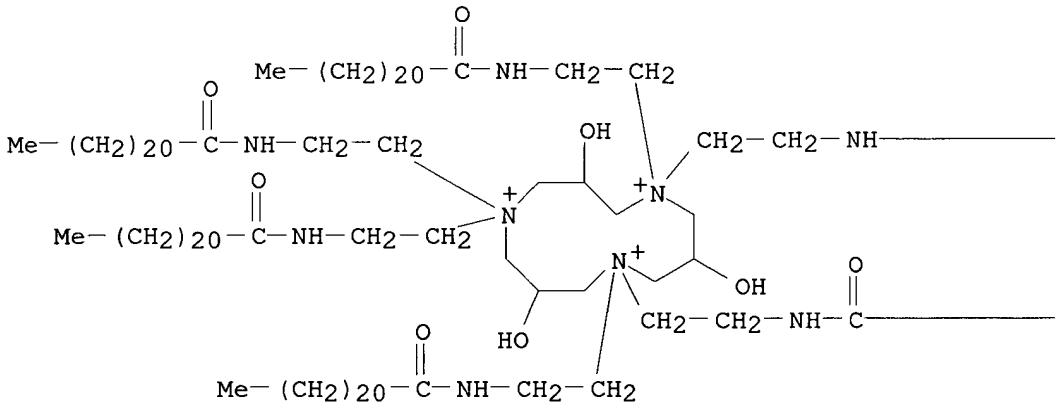
L20 ANSWER 26 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:752089 CAPLUS
DOCUMENT NUMBER: 132:3924
TITLE: Artificial leather sheets with good embossability and manufacture therewith
INVENTOR(S): Ikebukuro, Kazunari; Wakamatsu, Tomoyuki
PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11323742	A2	19991126	JP 1998-137300	19980520
PRIORITY APPLN. INFO.:			JP 1998-137300	19980520

AB The manufacture includes imparting a cationic surfactant onto a nonporous layer-covered fiber base layer and subjecting to the embossment treatment, where the nonporous layer consists of a diamine- or hydrazide-extended aliphatic or alicyclic polyurethane elastomer or a diol-extended MDI-type polyurethane elastomer. Coating a DMF solution of polyurethane elastomer (PUE) consisting of poly(ethylene adipate) glycol (I), 4,4'-MDI, ethylene glycol on a polyethylene film, coagulation in aqueous DMF, removing polyethylene film, and bonding the resulting porous film with a polyester fabric gave a base. Coating sequentially the base on the porous film with a polyurethane consisting of I, cyclohexylmethane-4,4'-diisocyanate, and isophoronediamine and PUE, treating with 1,5,9-Triazoniacyclododecane derivative cation [(C21H43CONHCH2CH2)2N+CH2CHOHCH2]3.3 Cl- and embossing gave a leather-like sheet with good appearance.

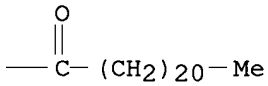
IT 137955-63-6
RL: TEM (Technical or engineered material use); USES (Uses)
(artificial leather sheets with good embossability and manufacture therewith)
RN 137955-63-6 CAPLUS
CN 1,5,9-Triazoniacyclododecane, 3,7,11-trihydroxy-1,1,5,5,9,9-hexakis[2-[(1-oxodocosyl)amino]ethyl]-, trichloride (9CI) (CA INDEX NAME)

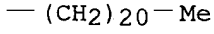
PAGE 1-A



● 3 Cl^-

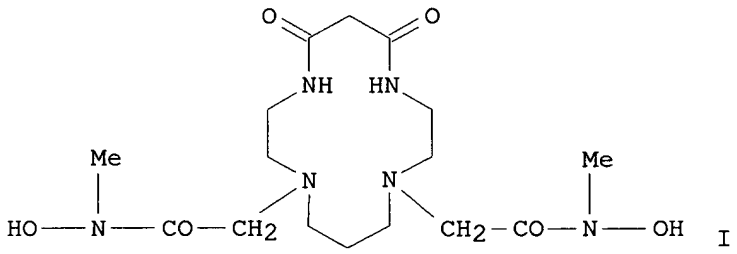
PAGE 1-B





L30 ANSWER 27 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:700785 CAPLUS
DOCUMENT NUMBER: 132:61413
TITLE: Molecular recognition of synthetic siderophore analogues: a study with receptor-deficient and fhu(A-B) deletion mutants of Escherichia coli
AUTHOR(S): Gaspar, Margarida; Santos, M. Amelia; Krauter, Katja; Winkelmann, Gunther
CORPORATE SOURCE: Centro de Quimica Estrutural, Complexo I, Instituto Superior Tecnico, Lisbon, 1049-001, Port.
SOURCE: BioMetals (1999), 12(3), 209-218
CODEN: BOMEEH; ISSN: 0966-0844
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

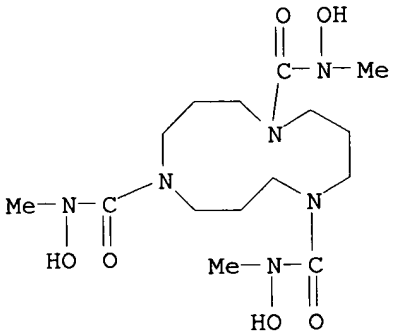
AB The biol. activity of six synthetic siderophore analogs [two dihydroxamates, two trihydroxamates, one tetrahydroxamate and one 3-hydroxy-4(1H)pyridinone] has been studied in Escherichia coli, Morganella morganii 13 and Proteus mirabilis 8993 strains by using growth promotion tests. Various transport-deficient mutants of E. coli were used to study the route of entry into gram-neg. bacteria. The results indicated that the synthetic hydroxamate compds. are transported via Fhu-mediated transport systems, although receptor specificity was low. This could be proven by using a delta (fhuA-B) E. coli mutant as a control in which growth promotion by natural hydroxamates was completely abolished, suggesting that a periplasmic binding-protein-dependent transport system (FhuB, C, D) is required for the transport of all synthetic ferric hydroxamate complexes. Although utilization of the synthetic hydroxamates was generally lower than that of the natural siderophores, differences in growth promotion could be detected. Highest activity was observed with the dihydroxamate DOCYDHAMA (I) ligand which supported growth at concns. <1 mM. In comparison with other polyamino-polyhydroxamate ligands studied, I has an extra diamide backbone that could be important for the interaction with the receptors or with FhuD. The synthetic trihydroxamate and tetrahydroxamate ligands showed a relatively low siderophore activity. Studies with Proteus and Morganella in the presence of increasing bipyridyl concns. showed a decreased growth promotion with the synthetic ferric hydroxamates, suggesting the involvement of a reduction step during iron mobilization or an increased toxicity of bipyridyl. This was not observed in the case of the 3-hydroxy-4(1H)pyridinone where bipyridyl had no effect.

IT 169386-06-5
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL

(Biological study); PROC (Process)
(mol. recognition of synthetic siderophore analogs studied with transport-deficient mutants of Escherichia coli)

RN 169386-06-5 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxamide, N,N',N''-trihydroxy-N,N',N''-trimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 28 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:631224 CAPLUS
DOCUMENT NUMBER: 131:279208
TITLE: Methine compound for silver halide photographic material
INVENTOR(S): Kato, Takashi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 23 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

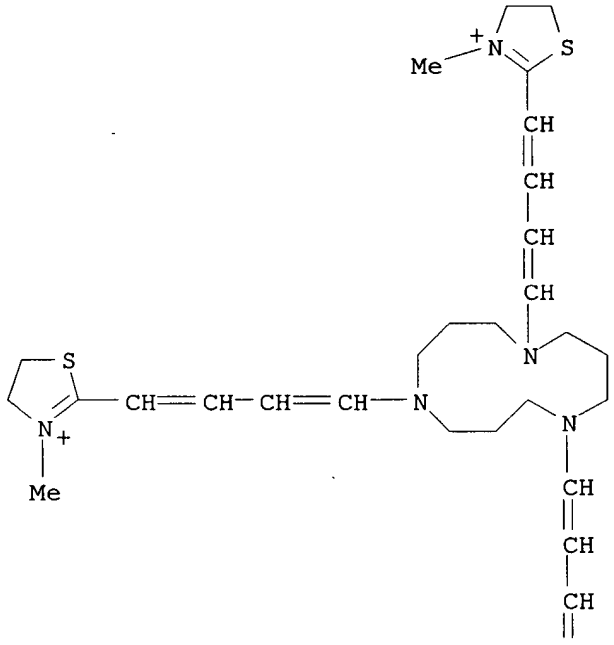
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11269398	A2	19991005	JP 1998-70936	19980319
PRIORITY APPLN. INFO.:			JP 1998-70936	19980319

AB The methine compound of a polymer hemicyanine has structure H1-A1-(-H2-A2-)q1-H3(H1-3 = hemicyanine dye; A1-2 = connecting group; q1 = 2-10,000 integer). The methine compound provides the improved sensitivity.

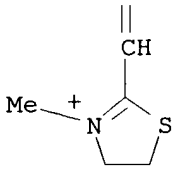
IT 245342-46-5
RL: TEM (Technical or engineered material use); USES (Uses)
(methine compound for silver halide photog. material)

RN 245342-46-5 CAPLUS
CN Thiazolium, 2,2',2''-(1,5,9-triazacyclododecane-1,5,9-triyltri-1,3-butadiene-4,1-diyl)tris[4,5-dihydro-3-methyl-, tribromide (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



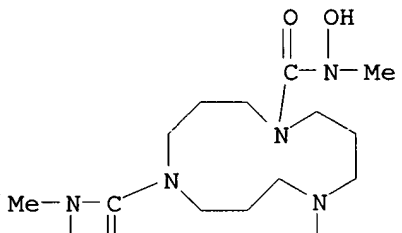
● 3 Br^-

L30 ANSWER 29 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:475681 CAPLUS
DOCUMENT NUMBER: 131:308148
TITLE: Polyamino-polyhydroxamic acids as siderophore analogs
AUTHOR(S): Santos, M. Amelia
CORPORATE SOURCE: Centro de Quimica Estrutural, Instituto Superior Tecnico, Lisbon, 1049-001, Port.
SOURCE: Monograph Series of the International Conferences on Coordination Chemistry held periodically at Smolenice in Slovakia (1999), 4(Coordination Chemistry at the Turn of the Century), 327-332
CODEN: MSICF5; ISSN: 1335-308X
PUBLISHER: Slovak Technical University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

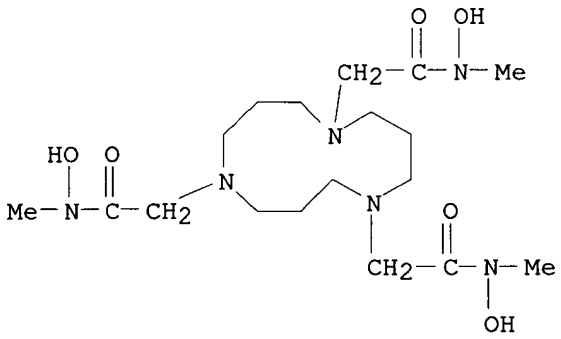
AB This paper presents a synopsis of the study of a set of polyamino-polyhydroxamate ligands as potential analogs of naturally occurring hydroxamate siderophores. They all have a cyclic (or macrocyclic) polyamine backbone with two or three hydroxamate pendant groups attached to the amine sites. Most of them are biol. active. They have been prepared by procedures which are schematically presented herein. Particular emphasis is devoted to their interaction with iron(III), namely what concerns the stability of the ferric complexes (Fe2L3 or FeL), their redox potentials, and the speciation at physiol. pH. Proposed structures of the dimeric complexes are supported by mol. modeling calcns. A summary of the in vivo studies is also presented. Comparison between the properties of the iron complexes and some siderophores is also made.

IT 169386-06-5P 247912-38-5P
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(polyamino-polyhydroxamic acids as siderophore analogs)

RN 169386-06-5 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxamide, N,N',N''-trihydroxy-N,N',N''-trimethyl- (9CI) (CA INDEX NAME)



RN 247912-38-5 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triacetamide, N,N',N''-trihydroxy-N,N',N''-trimethyl- (9CI) (CA INDEX NAME)



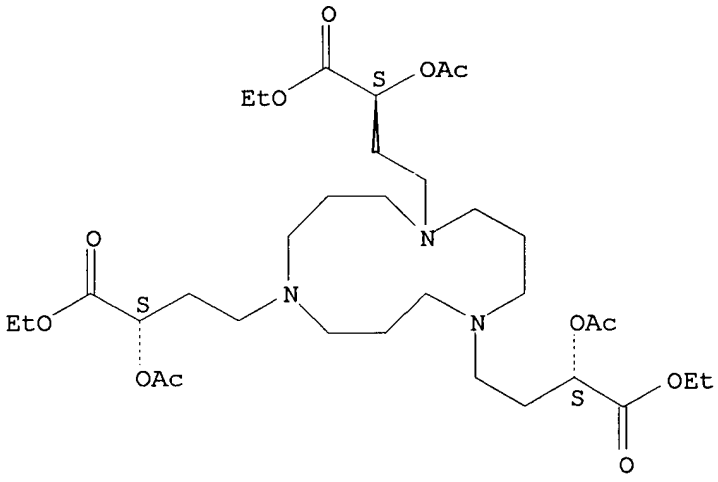
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 30 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:429230 CAPLUS
DOCUMENT NUMBER: 131:199688
TITLE: Synthesis of new triazamacrocycles N-functionalized with α-(S)-hydroxycarboxylic acid pendant-arms
AUTHOR(S): Delagrange, Samuel; Nepveu, Francoise
CORPORATE SOURCE: Laboratoire de Synthese, Physico-Chimie et Radiobiologie, Universite Paul Sabatier, Toulouse, 31062, Fr.
SOURCE: Tetrahedron Letters (1999), 40(27), 4989-4992
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis of two new macrocyclic ligands, N,N',N"-tris[2(S)-hydroxybutyric acid]-1,4,7-triazacyclononane [i.e., (S,S,S)-hexahydro-α,α',α''-trihydroxy-1H-1,4,7-triazonine-1,4,7-tributanoic acid] and N,N',N"-tris[2(S)-hydroxybutyric acid]-1,5,9-triazacyclododecane [i.e., (S,S,S)-hexahydro-α,α',α''-trihydroxy-1,5,9-triazacyclododecane-1,5,9-tributanoic acid] was reported. Each macrocycle bears three L-lactate-like pendant arms. Starting from L-malic acid, the absolute configuration of the α-(S)-hydroxy acid was kept along the synthesis leading to pure (S,S,S) enantiomers.

IT 241486-66-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of trihydroxytriazoninetributyrate and trihydroxytriazacyclododecanetributyrate)
RN 241486-66-8 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tributanoic acid, α,α',α''-tris(acetyloxy)-, triethyl ester, (αS,α'S,α''S)- (9CI) (CA INDEX NAME)

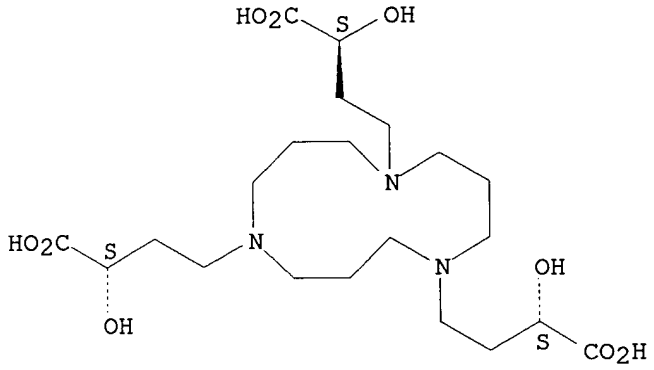
Absolute stereochemistry.



IT 241486-68-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of trihydroxytriazoninetributyrate and

trihydroxytriazacyclododecanetributyrate)
RN 241486-68-0 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tributanoic acid, α,α',α''-trihydroxy-, (αS,α'S,α''S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 31 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:420940 CAPLUS
DOCUMENT NUMBER: 131:74106
TITLE: Catalyst for olefin polymerization
INVENTOR(S): Sakai, Tatsuya
PATENT ASSIGNEE(S): JSR Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

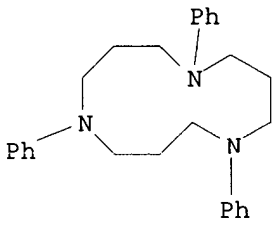
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11181013	A2	19990706	JP 1997-366004	19971224
PRIORITY APPLN. INFO.:			JP 1997-366004	19971224

OTHER SOURCE(S): MARPAT 131:74106

AB Title catalyst for homopolymn. and copolymn. of polar olefins or cycloolefins comprises (I) a transition metal (vanadium, niobium, tantalum, molybdenum, tungsten, manganese, iron, cobalt, nickel, ruthenium, rhodium, palladium, iridium or platinum) coordinated with a cyclic compound having ≥2 nitrogen atoms in saturated bonds with carbon atoms, (II) an organo-aluminum compound (R1)aALZ3-a, wherein R1 is C1-20 hydrocarbon, Z is H, halogen, or alkoxy, 0<a≤3, and (III) an ionic compound Thus, 1-hexene and ethylene were polymerized in the presence of methylaluminoxane and 1,5,9-triazadodecanyl tantalum dichloride synthesized from 1,5,9-triazadodecane and tantalum pentachloride to give a copolymer with mol. weight 90,000, mol. weight distribution 2.52, and hexene content 31%.

IT 228997-91-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(catalyst for olefin polymerization)

RN 228997-91-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-triphenyl- (9CI) (CA INDEX NAME)

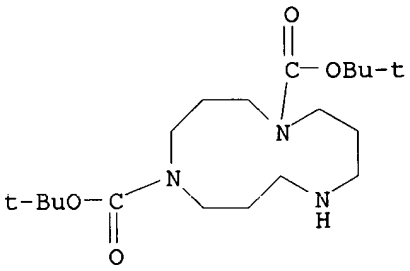


L30 ANSWER 32 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:411134 CAPLUS
DOCUMENT NUMBER: 131:138432
TITLE: Synthesis, crystal structure and magnetic properties of a new dicopper(II) complex with a bis(macrocyclic) ligand
AUTHOR(S): Bu, Xian-He; Chen, Wei; Zhang, Ruo-Hua; Chen, Rong-Ti
CORPORATE SOURCE: Dep. Chem., Nankai Univ., Tianjin, 300071, Taiwan
SOURCE: Huaxue Xuebao (1999), 57(6), 627-634
CODEN: HHHPA4; ISSN: 0567-7351
PUBLISHER: Kexue Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB A new binuclear Cu(II) complex, [Cu2L.Br2]Br·H2O, where L is a new binucleating macrocyclic ligand 2,6-bis(1,5,9-triazacyclododecan-9-ylmethyl)benzoate, was prepared and characterized by x-ray crystallog. Crystal data: monoclinic, space group P21/c, a 1.1666(2), b 1.3541(3), c 2.2750(5) nm, β 99.38(3)°, Z = 4. The binuclear Cu(II) center ions are bridged by a μ-carboxyl group of L and separated by 0.5884 nm. Both of the Cu(II) ion centers are coordinated by three amine nitrogens of [12]aneN3 subunit and one O of the carboxyl group, as well as one bromide ion. The Cu(II) ion is in the trigonal bipyramid environment. Variable temperature magnetic susceptibility studies indicate that there exists intramol. antiferromagnetic coupling (J = -22.49cm-1) between the two Cu(II) centers.

IT 174192-40-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of copper bis(triazacyclododecanylmethyl)benzoate dinuclear complex)

RN 174192-40-6 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

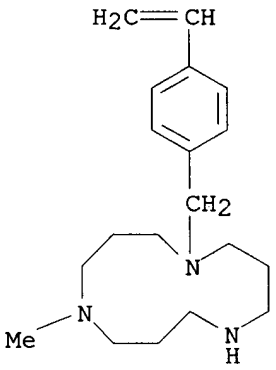


L30 ANSWER 33 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:357902 CAPLUS
DOCUMENT NUMBER: 131:214628
TITLE: Efficient syntheses of polymerizable pendant arm azamacrocycles and formation of poly(vinylbenzyltriazacyclododecane)
AUTHOR(S): Long, Nicholas J.; Parker, David G.; Speyer, Paul R.; White, Andrew J. P.; Williams, David J.
CORPORATE SOURCE: Department of Chemistry, Imperial College of Science, Technology and Medicine, South Kensington, London, SW7 2AY, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (12), 1621-1624
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

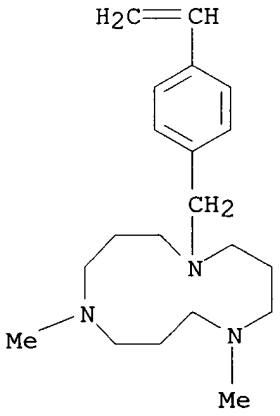
AB Synthetic routes to a number of metal-free triazacyclododecane derivs. featuring the unsym. incorporation of polymerizable pendant side arms such as vinylbenzene and methacrylate were developed. The structure of a nitrate salt of the vinylbenzene-substituted species was determined by single crystal X-ray diffraction and the first polymer-bound triazamacrocycles formed via free-radical polymerization of a metal-free macrocycle-containing monomer.

IT 243670-33-9P 243670-34-0P 243670-35-1P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(efficient syntheses of polymerizable pendant arm azamacrocycles and formation of poly(vinylbenzyltriazacyclododecane))

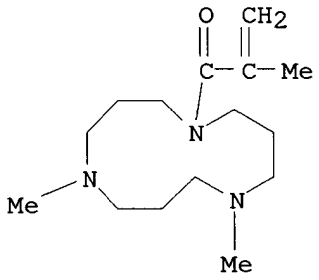
RN 243670-33-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 1-[(4-ethenylphenyl)methyl]-5-methyl- (9CI) (CA INDEX NAME)



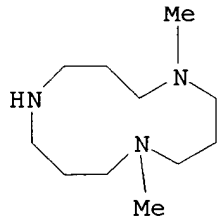
RN 243670-34-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 1-[(4-ethenylphenyl)methyl]-5,9-dimethyl- (9CI) (CA INDEX NAME)



RN 243670-35-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-dimethyl-9-(2-methyl-1-oxo-2-propenyl)- (9CI) (CA INDEX NAME)



IT 139258-69-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(efficient syntheses of polymerizable pendant arm azamacrocycles and formation of poly(vinylbenzyltriazacyclododecane))
RN 139258-69-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-dimethyl- (9CI) (CA INDEX NAME)



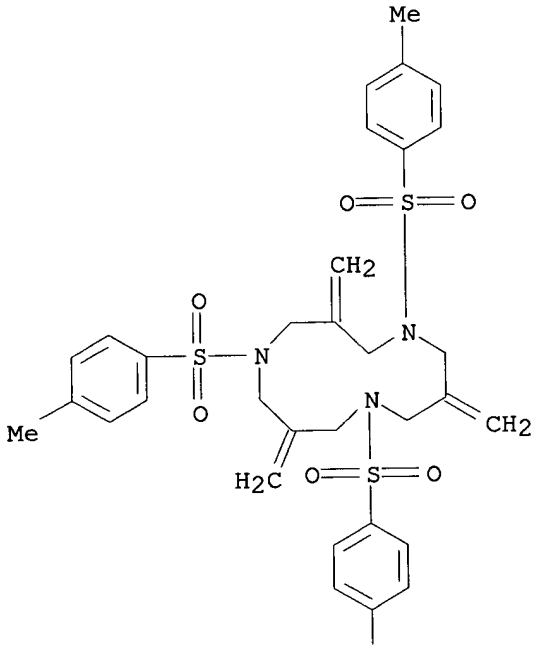
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 34 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:757792 CAPLUS
DOCUMENT NUMBER: 130:153220
TITLE: Palladium(0)-catalyzed allylation of highly acidic and non-nucleophilic arenesulfonamides, sulfamide, and cyanamide.II. Formation of medium and large heterocycles
AUTHOR(S): Cerezo, Silvia; Cortes, Jordi; Lopez-Romero, Juan-Manuel; Moreno-Manas, Marcial; Parella, Teodor; Pleixats, Roser; Roglans, Anna
CORPORATE SOURCE: Department of Chemistry, Universitat Autonoma de Barcelona, Barcelona, 08193, Spain
SOURCE: Tetrahedron (1998), 54(49), 14885-14904
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:153220

AB Arenesulfonamides, cyanamide derivs., and sulfamide derivs. react with allylic bis(carbonates) under Pd(0)-catalysis to afford medium and large unsatd. heterocycles instead of three and/or five-membered ring compds. Stable 15-membered palladium-containing rings were also isolated from arenesulfonamides with three trans olefinic systems coordinated to the metal. NMR and MALDI-TOF MS expts. were used for structure elucidation. Suitable hydrogenation conditions to give the saturated macrocycles were found.

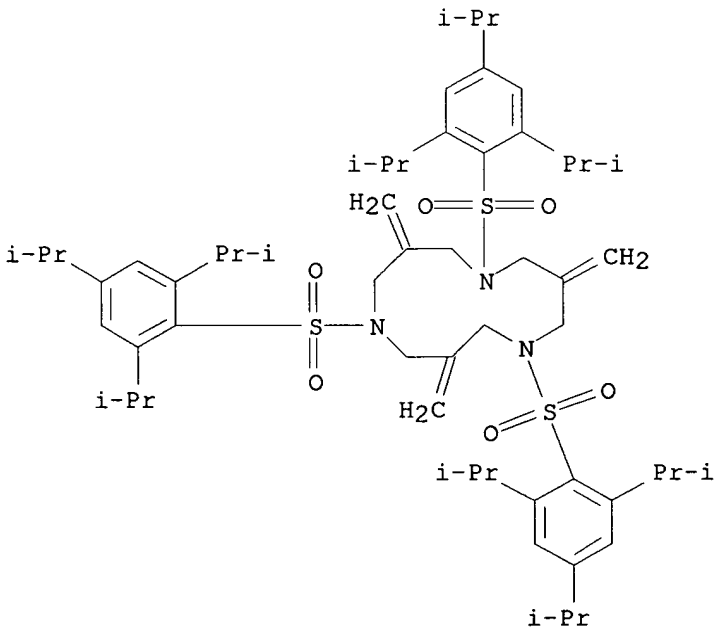
IT 130927-35-4P 219839-43-7P 219839-47-1P
219839-49-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 130927-35-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

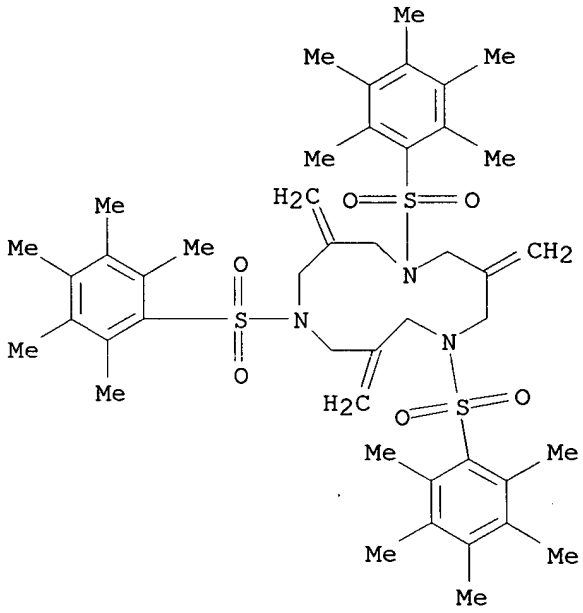


PAGE 2-A

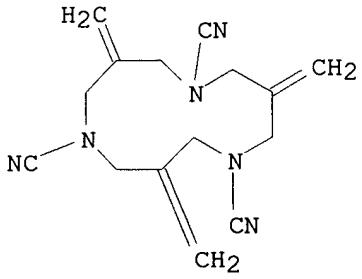
RN 219839-43-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[[2,4,6-tris(1-methylethyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



RN 219839-47-1 CAPLUS
CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[(pentamethylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 219839-49-3 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarbonitrile, 3,7,11-tris(methylene)-(9CI) (CA INDEX NAME)

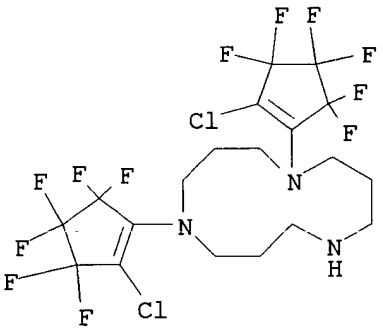


REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

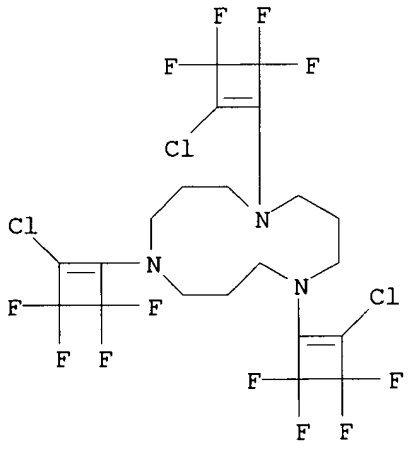
L10 ANSWER 35 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:605672 CAPLUS
DOCUMENT NUMBER: 129:290121
TITLE: Reactions of Dichloroperfluorocycloalkenes with Triazamacrocyclic Amines
AUTHOR(S): Gupta, O. D.; Chen, Jianguo; Kirchmeier, Robert L.; Shreeve, Jean'ne M.
CORPORATE SOURCE: Department of Chemistry, University of Idaho, Moscow, ID, 83844-2343, USA
SOURCE: Inorganic Chemistry (1998), 37(20), 5342-5345
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 1,2-Dichlorotetrafluorocyclobutene (A) and 1,2-dichlorohexafluorocylopentene-1 (B) reacted with triazamacrocyclic amines 1,4,8-triazacycloundecane (1) and 1,5,9-triazacyclo-dodecane (2) at 80° with stoichiometric amts. of NEt3 in benzene. Cycloalkene A formed a 2:1 product 1,5-bis(chlorotetrafluorocyclobutenyl)-1,5,8-triazacycloundecane (3) with 1 and a 3:1 product 1,5,9-tris(chlorotetrafluorocyclobutenyl)-1,5,9-triazacyclododecane (4) with 2. B formed only 2:1 products 1,5-Bis(chlorohexafluorocyclopentenyl)-1,5,8-triazacycloundecane (5) and 1,5-Bis(chlorohexafluorocyclopentenyl)-1,5,9-triazacyclododecane (6) with 1 and 2, resp. The crystal structures of 3 and 4 were determined by single-crystal x-ray diffraction.

IT 214191-81-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation from reactions of dichloroperfluorocycloalkenes with triazamacrocyclic amines)
RN 214191-81-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis(2-chloro-3,3,4,4,5,5-hexafluoro-1-cyclopenten-1-yl)- (9CI) (CA INDEX NAME)



IT 214191-79-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation from reactions of dichloroperfluorocycloalkenes with triazamacrocyclic amines and crystal structure)
RN 214191-79-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris(2-chloro-3,3,4,4-tetrafluoro-1-cyclobuten-1-yl)- (9CI) (CA INDEX NAME)

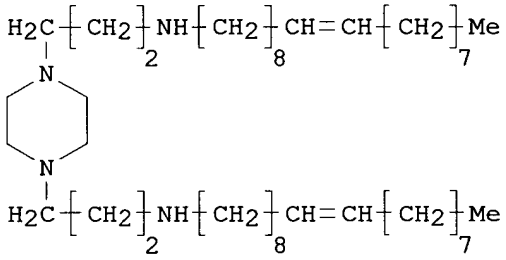


REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 36 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:263206 CAPLUS
DOCUMENT NUMBER: 128:266964
TITLE: Process of transfecting a cell with a polynucleotide mixed with an amphipathic compound and a DNA-binding protein
INVENTOR(S): Wolff, Jon A.; Fritz, Jeffery; Budker, Vladimir; Hagstrom, James
PATENT ASSIGNEE(S): Mirus Corporation, USA
SOURCE: U.S., 16 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5744335	A	19980428	US 1995-530598	19950919
US 6180784	B1	20010130	US 1998-20566	19980117
PRIORITY APPLN. INFO.:			US 1995-530598	A3 19950919
OTHER SOURCE(S):	MARPAT 128:266964			

GI



I

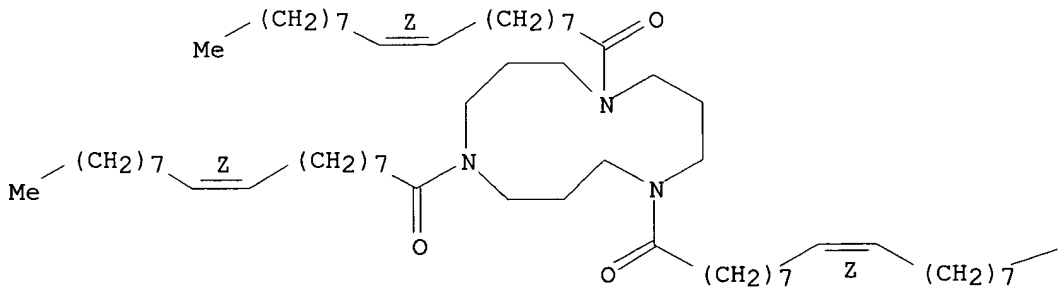
AB Transfection of a cell is accomplished using with a polynucleotide mixed with one or more amphipathic compds. and a DNA-binding protein, especially a histone such as histones H1, H2A, or H2B. The DNA-binding protein may be fused to a nuclear localization signal peptide. Exemplary and preferred amphipathic compds. are cationic amphipathic compds. I was synthesized in 70% yield by reacting 1,4-bis(3-aminopropyl)piperazine with oleoyl chloride and reducing the intermediate with LiAlH4 in THF. Histone H1 was found to increase the transfection efficiency of I 16.1-fold. I/H1 reagent has a greater transfection efficiency and less cellular toxicity then LipofectAmine, which is useful in gene therapy.

IT 205596-17-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(amphipathic compds. for transfecting cells and their syntheses)

RN 205596-17-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris(1-oxo-9-octadecenyl)-, (all-Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

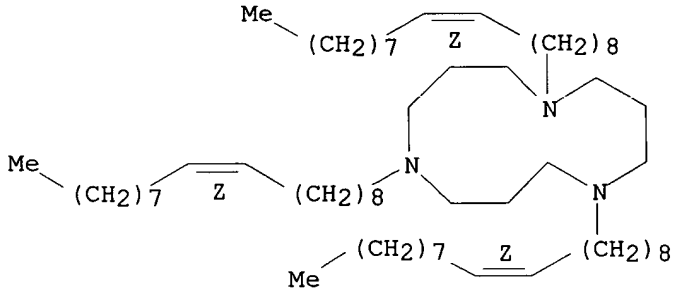


PAGE 1-B

Me

IT 205596-16-3P
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cell transfection with polynucleotide mixed with amphipathic compound and DNA-binding protein)
RN 205596-16-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tri-9-octadecenyl-, (all-Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 37 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:795802 CAPLUS
DOCUMENT NUMBER: 128:93621
TITLE: The azamacrocyclic derivatives of H4Ru4(CO)12 and their reactivity with CO and catalytic activity in the methanol carbonylation and in the water-gas shift reaction
AUTHOR(S): Kallinen, K. O.; Pakkanen, T. T.; Pakkanen, T. A.
CORPORATE SOURCE: P.O. Box, University of Joensuu, Department of Chemistry, Joensuu FIN-80101, 111, Finland
SOURCE: Journal of Organometallic Chemistry (1997), 547(2), 319-327
CODEN: JORCAI; ISSN: 0022-328X
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English

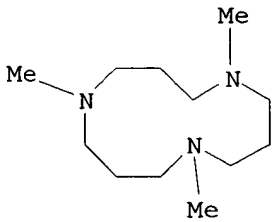
AB The reactions of H4Ru4(CO)12 with cyclic triazaligands result in the formation of [LH]+[H3Ru4(CO)12]- salts, (L=1,4,7-triazacyclononane, 1,4,7-trimethyl-1,4,7-triaza-cyclononane, 1,5,9-triazacyclododecane and 1,5,9-trimethyl-1,5,9-triazacyclo-dodecane). The compds. were synthesized by refluxing H4Ru4(CO)12 in hexane followed by precipitation with the corresponding ligand. This is a convenient direct single-step synthetic route to produce [H3Ru4(CO)12]- ion with a high yield. The compds. have been characterized by elemental anal. and spectroscopic measurements. In the 1H NMR spectra they showed a fluxional behavior. Reactivity towards CO at elevated temperature, and the catalytic activity of the new compds. in the water-gas shift reaction (WGSR) and in the carbonylation of methanol, have been discussed.

IT 201154-76-9P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(azamacrocyclic derivs. of H4Ru4(CO)12 and their reactivity with CO and catalytic activity in the methanol carbonylation and in the water-gas shift reaction)

RN 201154-76-9 CAPLUS
CN Ruthenium, dodecacarbonyltetra-μ-hydrotetra-, tetrahedro, compd. with 1,5,9-trimethyl-1,5,9-triazacyclododecane (1:1) (9CI) (CA INDEX NAME)

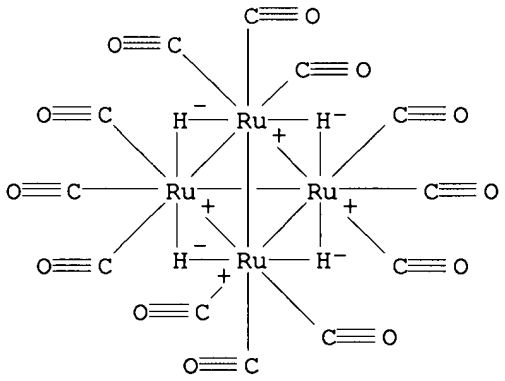
CM 1

CRN 133256-59-4
CMF C12 H27 N3



CM 2

CRN 34438-91-0
CMF C12 H4 O12 Ru4
CCI CCS



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

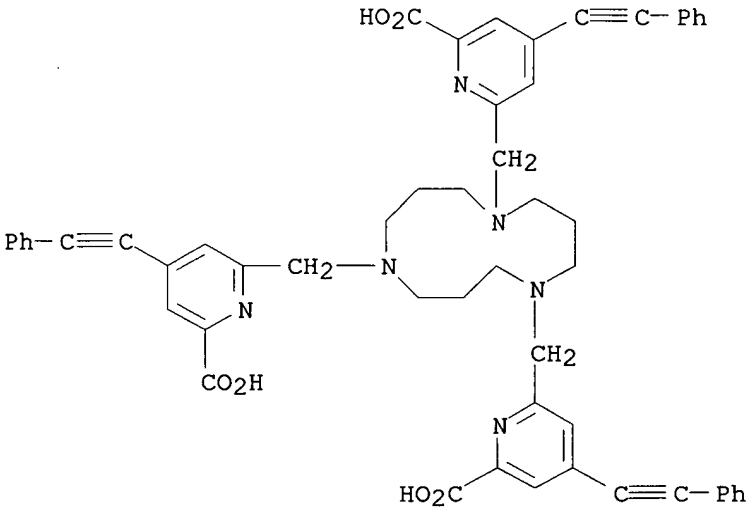
L30 ANSWER 38 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:753649 CAPLUS
DOCUMENT NUMBER: 128:121166
TITLE: Evaluation of solution structures of highly luminescent europium(III) chelates by using laser induced excitation of the 7F0→5D0 transition
AUTHOR(S): Latva, Martti; Takalo, Harri; Mukkala, Veli-Matti; Kankare, Jouko
CORPORATE SOURCE: Department of Chemistry, University of Turku, Turku, FIN-20014, Finland
SOURCE: Inorganica Chimica Acta (1998), 267(1), 63-72
CODEN: ICHAA3; ISSN: 0020-1693
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Solution structures of 13 Eu(III) chelates were examined by using laser induced excitation of the 7F0→5D0 transition. Remarkable variations in the 7F0→5D0 excitation spectra of 2,2',2'',2'''-{[aryl]bis(methylenenitrilo)}tetrakis(acetic acid) complexes of Eu(III) are observed depending on the denticity of the ligand and the number and character of the coordinated N atoms. The evaluation of the structures is made from the energy of the 7F0→5D0 excitation transition of Eu(III) because the 7F0→5D0 transition energy is dependent on the number and type of coordinating atoms in the 1st coordination sphere of Eu(III). Addnl. information about the structures is obtained by measuring the excited-state lifetimes of the Eu(III) chelates. The 7F0→5D0 transition energy shifts always an equal amount to lower energies due to the coordination of a certain group or atom. The energies of the 7F0→5D0 excitation transitions are also used to calculate these nephelauxetic shift parameters for coordinated N heteroatoms in the 2,2',2'',2'''-{[4-(phenylethynyl)pyridine-2,6-diyl]bis-(methylenenitrilo)}tetrakis(acetic acid) (3), 2,2',2'',2'''-[(2,2'-bipyridine-6,6'-diyl)bis-(methylenenitrilo)]tetrakis(acetic acid) (4), 2,2',2'',2'''-[(2,2':6'2''-terpyridine-6,6''-diyl)bis(methylenenitrilo)]tetrakis(acetic acid) (5), 2,2',2'',2'''-{[6,6'-(pyrazole-1,3-diyl)-bis(pyridine)-2,2'-diyl]bis(methylenenitrilo)}tetrakis(acetic acid) (7), 2,2',2'',2'''-{[6,6'-(thiazole-2,4-diyl)bis(pyridine)-2,2'-diyl]-bis(methylenenitrilo)}tetrakis(acetic acid) (8) and 2,2',2'',2'''-{[2,2'-(pyridine-2,6-diyl)bis(thiazole)-4,4'-diyl]bis-(methylenenitrilo)}-tetrakis(acetic acid) (9) complexes. The variation in the shift parameters of the N heteroatoms probably is due to the different distances between the N heteroatoms and Eu(III) ions.

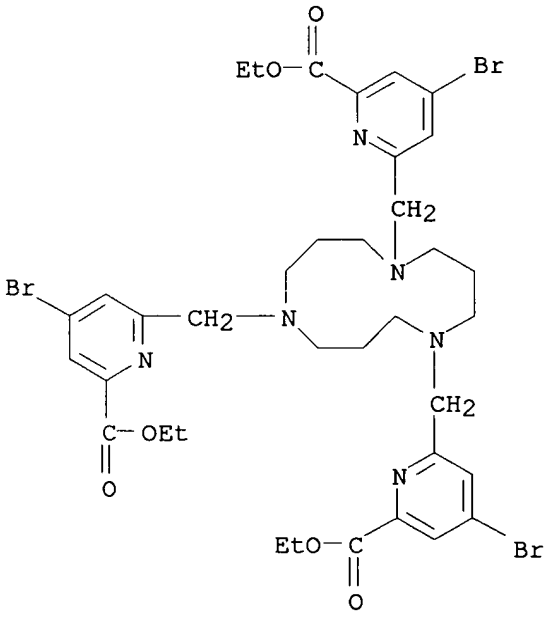
IT 201748-91-6D, europium complexes
RL: PRP (Properties)
(evaluation of solution structures of highly luminescent europium(III) chelates by using laser induced excitation of 7F0→5D0 transition)

RN 201748-91-6 CAPLUS
CN 2-Pyridinecarboxylic acid, 6,6',6''-[1,5,9-triazacyclododecane-1,5,9-triyltris(methylene)]tris[4-(phenylethynyl)- (9CI) (CA INDEX NAME)



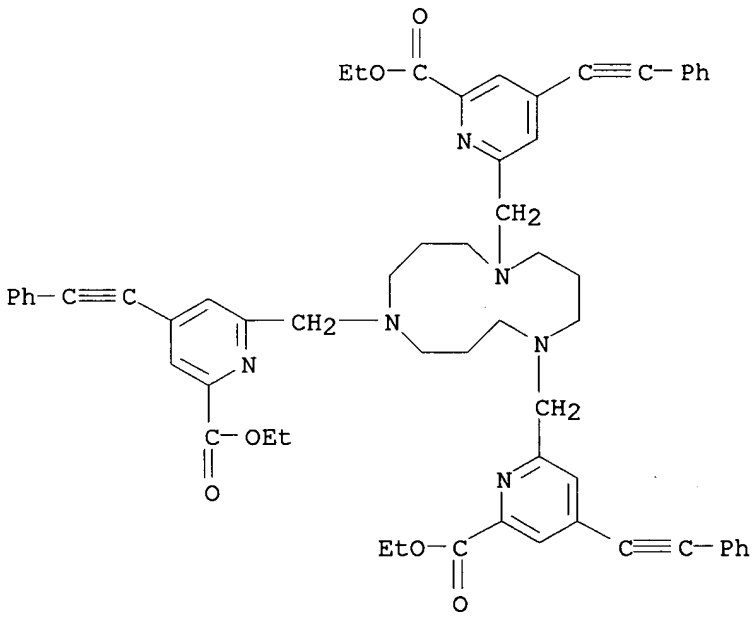
IT 201748-92-7P 201748-93-8P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(evaluation of solution structures of highly luminescent europium(III) chelates by using laser induced excitation of 7F0→5D0 transition)

RN 201748-92-7 CAPLUS
CN 2-Pyridinecarboxylic acid, 6,6',6''-[1,5,9-triazacyclododecane-1,5,9-triyltris(methylene)]tris[4-bromo-, triethyl ester (9CI) (CA INDEX NAME)



RN 201748-93-8 CAPLUS
CN 2-Pyridinecarboxylic acid, 6,6',6''-[1,5,9-triazacyclododecane-1,5,9-

triyltris(methylene)]tris[4-(phenylethynyl)-, triethyl ester (9CI) (CA INDEX NAME)



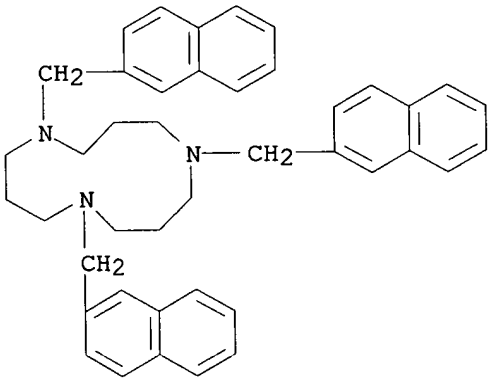
REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 39 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:589536 CAPLUS
DOCUMENT NUMBER: 127:248091
TITLE: Synthesis and properties of N,N',N"-tris(1-naphthylmethyl)-1,5,9-triazacyclododecane
AUTHOR(S): Kubo, Kanji; Yamamoto, Emi; Sakurai, Tadamitsu
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Kanagawa University, Yokohama, 221, Japan
SOURCE: Heterocycles (1997), 45(8), 1457-1461
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB N,N'-Bis(1-naphthylmethyl)piperazine and N,N',N"-tris(1-naphthylmethyl)-1,5,9-triazacyclododecane were found to display unique photophys. properties for the guest salts. These guest salts enhanced the host emission remarkably by the inhibition of intramol. exciplex formation and then quenched the emission by photoinduced electron transfer from the counter anion to the naphthalene chromophore in the presence of high concns. of the salts.

IT 195883-54-6P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tris(naphthylmethyl)triazacyclododecane and bis(naphthylmethyl)piperazine)

RN 195883-54-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris(2-naphthalenylmethyl)- (9CI) (CA INDEX NAME)



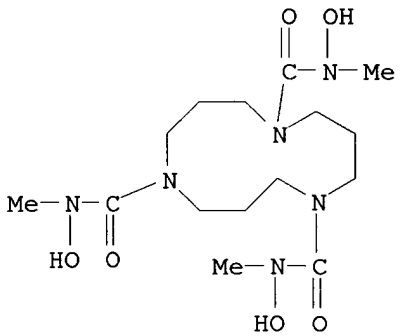
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L80 ANSWER 40 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:355708 CAPLUS
DOCUMENT NUMBER: 127:77654
TITLE: Iron release mechanism in a trihydroxamate siderophore analog. Kinetics and effect of pH
AUTHOR(S): Santos, M. A.; Bento, C.; Esteves, M. A.; Farinha, J. P. S.; Martinho, J. M. G.
CORPORATE SOURCE: Centro de Quimica Estrutural, Complexo I, Instituto Superior Tecnico, 1096, Lisbon, Port.
SOURCE: Inorganica Chimica Acta (1997), 258(1), 39-46
CODEN: ICHAA3; ISSN: 0020-1693
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In view of the potential importance of the siderophore analog DOTRMAHA as an iron carrier in biol. systems, we have decided to study the mechanism and kinetics of iron release from the ferric DOTRMAHA complex to EDTA. The kinetics of the iron(III) exchange was monitored by UV-Vis absorption spectroscopy at the wavelength maximum of the iron(III) trihydroxamate complex. The decay of the complex absorbance with time is described as a sum of two exponentials plus a constant term. The mechanism of the exchange reaction is examined under conditions of varying concns. of the competing ligand and the hydrogen ion. The kinetics reveal pseudo-first order dependence of rate constant(s) on the EDTA concentration Furthermore, pH dependence studies show that the exchange reaction is accelerated with increasing acidity of the medium. The results are mechanistically interpreted by a kinetic scheme involving two parallel pathways for the iron exchange: one is a bimol. process involving the direct attack of the EDTA on the ferric siderophore analog complex; the other involves initially the protonation of the complex followed by a rapid attack of the competing ligand. The set of kinetic data presented here is further rationalized in terms of known coordination and structural features of the DOTRMAHA ligand as well as the corresponding ferric complex, and compared with available data of some naturally occurring siderophores and synthetic analogs.

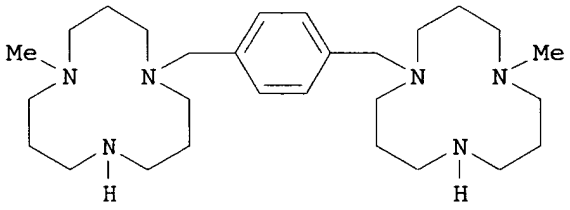
IT 169386-06-5, DOTRMAHA
RL: BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(iron release mechanism in a trihydroxamate siderophore analog, kinetics and effect of pH)

RN 169386-06-5 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxamide, N,N',N''-trihydroxy-N,N',N''-trimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 41 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:190886 CAPLUS
DOCUMENT NUMBER: 126:293343
TITLE: Synthesis and characterization of a new series of [12]aneN3 type macrocycles. Structures of two protonated metal-free ligands
AUTHOR(S): Hubsch-Weber, Patricia; Youinou, Marie-Therese
CORPORATE SOURCE: Lab. Chim. Metaux Transition Catalyse, Univ. Louis Pasteur, Strasbourg, 67000, Fr.
SOURCE: Tetrahedron Letters (1997), 38(11), 1911-1914
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

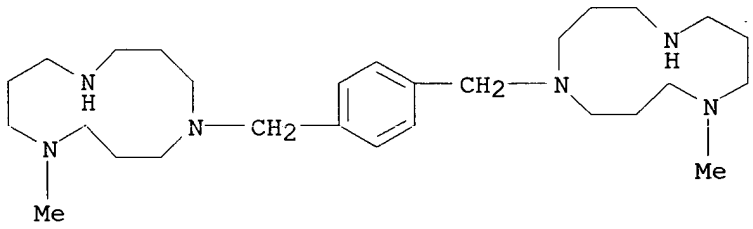


I

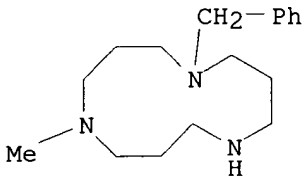
AB The synthesis of a family of monotopic and ditopic ligands possessing a [12]aneN3 synthon and different spacers, e.g., I, is described. The characterization of two of them by x-ray diffraction is also reported.

IT 189076-29-7P 189076-30-0P 189076-34-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of aneN3 macrocycles)

RN 189076-29-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,1'-[1,4-phenylenebis(methylene)]bis[5-methyl- (9CI) (CA INDEX NAME)

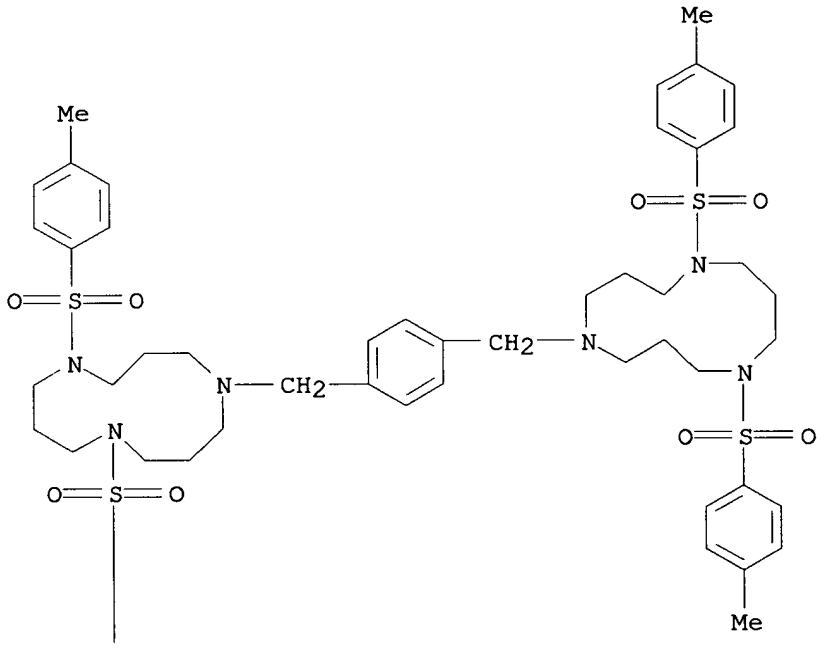


RN 189076-30-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 1-methyl-5-(phenylmethyl)- (9CI) (CA INDEX NAME)

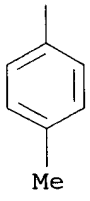


RN 189076-34-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,1'-[1,4-phenylenebis(methylene)]bis[5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L80 ANSWER 42 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:741489 CAPLUS
DOCUMENT NUMBER: 126:89764
TITLE: Macrocyclic triamines as linkers in two-armed receptors for peptides
AUTHOR(S): Iorio, Edward James; Still, W. Clark
CORPORATE SOURCE: Department Chemistry, Columbia University, New York, NY, 10027, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1996), 6(22), 2673-2676
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

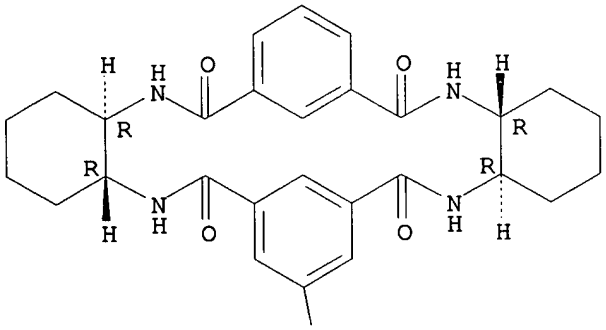
AB Com. available triazamacrocycles have been substituted with trimesic acid/1,2-diamine cyclooligomers to create a new class of sequence-selective receptors for peptides. Screening of these compds. against a 3375-member library of N-acetyl tripeptides revealed novel peptide-binding properties.

IT 185756-45-0P
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(preparation of macrocyclic triamines as linkers in two-armed receptors for peptides)

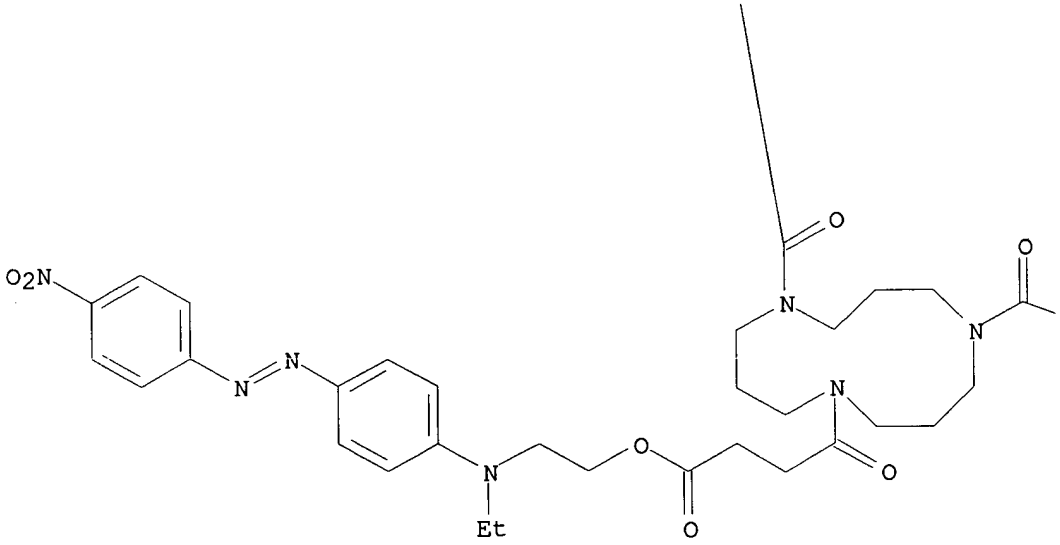
RN 185756-45-0 CAPLUS
CN 1,5,9-Triazacyclododecane-1-butanoic acid, 5,9-bis[(1,2,3,4,4a,5,6,12,13,13a,14,15,16,17,17a,18,19,25,26,26a-eicosahydro-6,12,19,25-tetraoxo-7,11:20,24-dimethenodibenzo[b,m][1,4,12,15]tetraazacyclodocosin-9-yl)carbonyl]-γ-oxo-, 2-[ethyl[4-[(4-nitrophenyl)azo]phenyl]amino]ethyl ester, [4aR-[4aR*,9(4aR*,13aR*,17aR*,26aR*),13aR*,17aR*,26aR*]]- (9CI) (CA INDEX NAME)

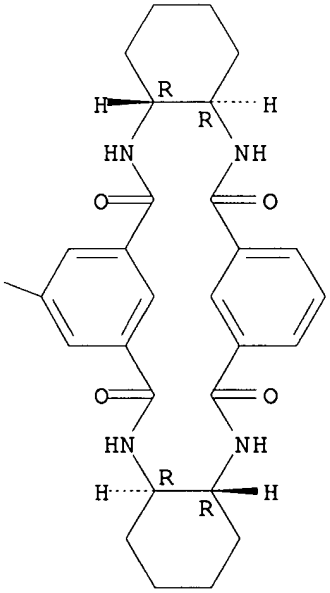
Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A



PAGE 2-A





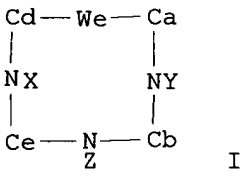
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L30 ANSWER 43 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:635114 CAPLUS
DOCUMENT NUMBER: 125:265995
TITLE: Antiviral triaza compounds and their preparation
INVENTOR(S): Bell, Thomas W.
PATENT ASSIGNEE(S): Research Foundation of State University of New York, USA
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9625167	A1	19960822	WO 1996-US2132	19960216
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5663161	A	19970902	US 1995-392550	19950217
CA 2211920	AA	19960822	CA 1996-2211920	19960216
AU 9651704	A1	19960904	AU 1996-51704	19960216
AU 701783	B2	19990204		
EP 809504	A1	19971203	EP 1996-908473	19960216
EP 809504	B1	20020515		
R: AT, BE, CH, DE, DK, FR, GB, IT, LI, NL, SE, IE				
CN 1181013	A	19980506	CN 1996-193110	19960216
JP 11500130	T2	19990106	JP 1996-525169	19960216
AT 217529	E	20020615	AT 1996-908473	19960216
US 6342492	B1	20020129	US 1997-894491	19970807

PRIORITY APPLN. INFO.: US 1995-392550 A2 19950217
WO 1996-US2132 W 19960216

OTHER SOURCE(S): MARPAT 125:265995
GI



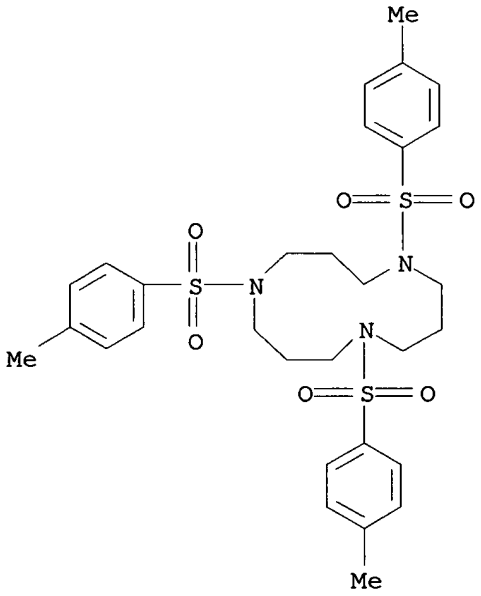
I

AB A method is disclosed for inhibiting viruses, in which a virus is contacted with an antiviral amount of I [W = bridge C with polar or nonpolar side group; X, Y = aromatic (aromatic = Ar (Ar = aromatic cyclic or aromatic heterocyclic ring of 5-7 members), Ar-sulfonyl, Ar-carboxy and Ar-alkyl), C1-10 alkyl, sulfonyl, carbonyl; Z = H, X, Y, C7-10 fused aryl; a, d, e = 0-10; b, c = 1-10]; the compds. are cyclic or acyclic and include sufficient Hydrogens for stable mols. Preparation of selected I is described, and activity against HIV and other viruses is presented.

IT 35980-67-7P 182316-06-9DP, acyl derivative
182316-06-9P 182316-08-1P 182316-10-5P
182316-12-7P 182316-15-0P 182316-17-2P
182316-19-4P 182316-20-7P 182316-21-8P
182316-22-9P 182316-25-2P 182316-27-4DP, acyl
derivative 182316-27-4P 182316-30-9P 182316-34-3P
182316-44-5P 182316-50-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antiviral triaza compound preparation and activity)

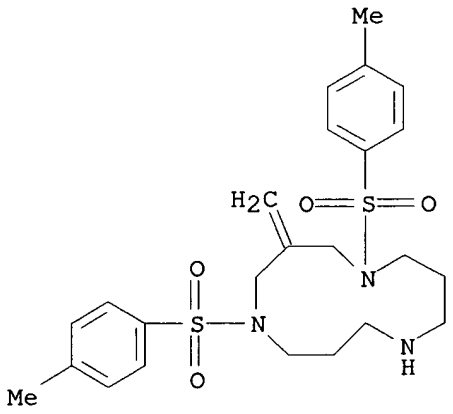
RN 35980-67-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

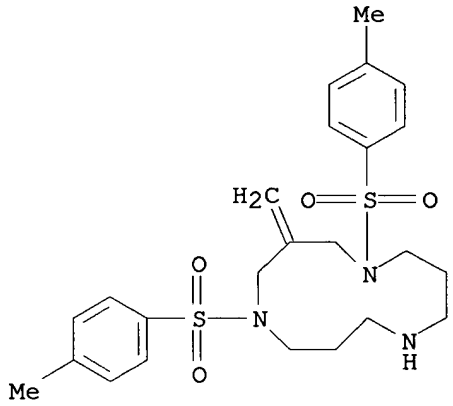


RN 182316-06-9 CAPLUS

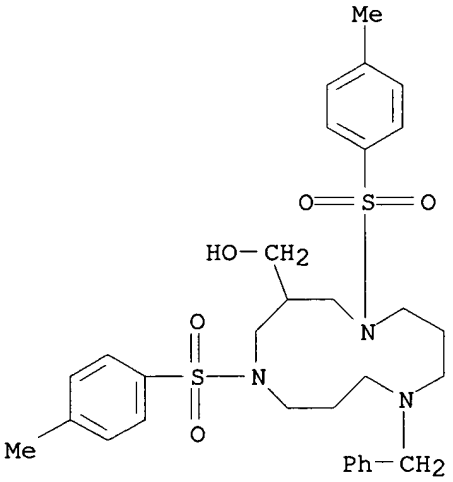
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



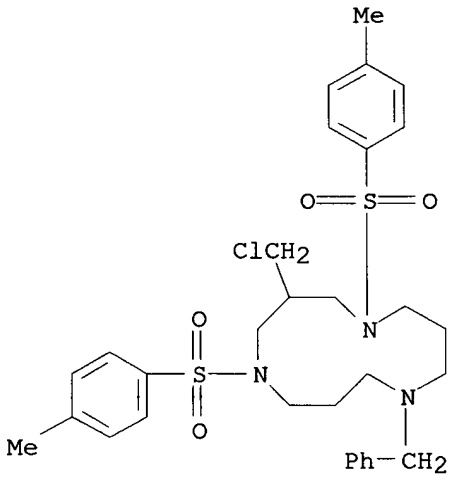
RN 182316-06-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-
(9CI) (CA INDEX NAME)



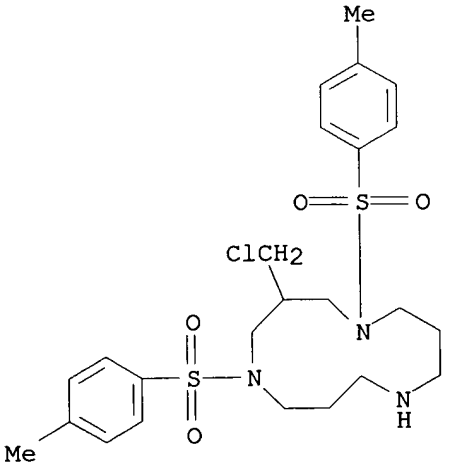
RN 182316-08-1 CAPLUS
CN 1,5,9-Triazacyclododecane-3-methanol, 1,5-bis[(4-methylphenyl)sulfonyl]-9-
(phenylmethyl)- (9CI) (CA INDEX NAME)



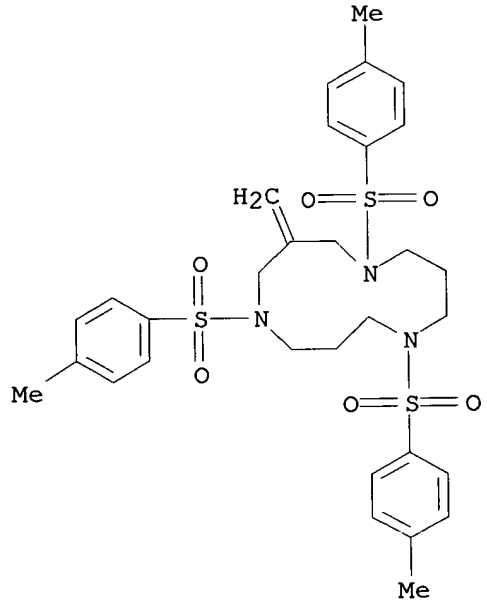
RN 182316-10-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 182316-12-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

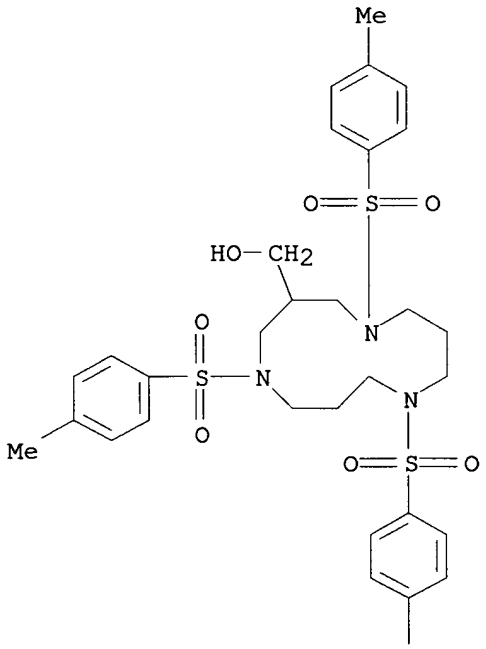


RN 182316-15-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 182316-17-2 CAPLUS
CN 1,5,9-Triazacyclododecane-3-methanol, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

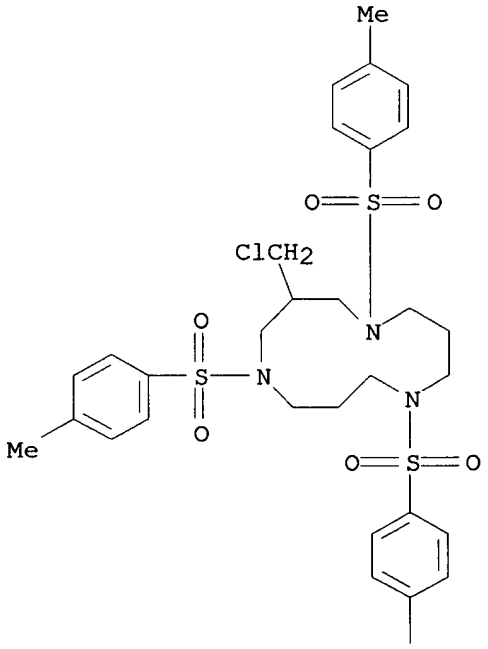
PAGE 1-A



PAGE 2-A

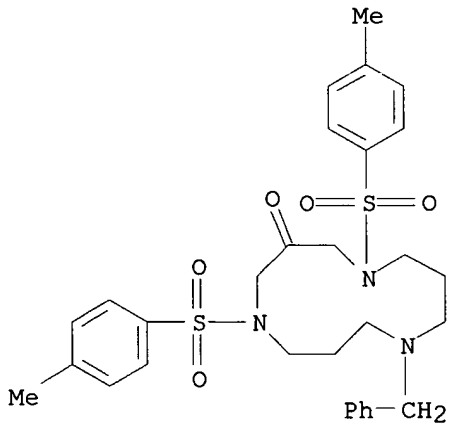
RN 182316-19-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-(chloromethyl)-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



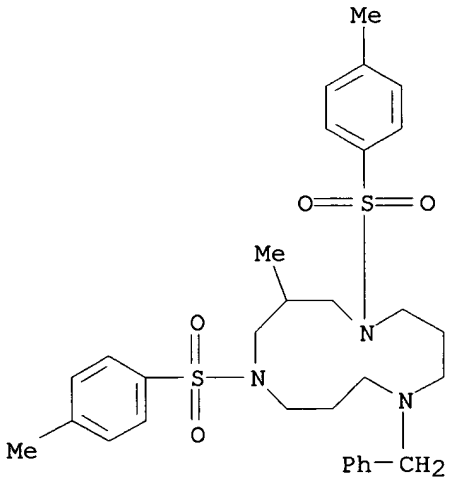
PAGE 2-A

RN 182316-20-7 CAPLUS
CN 1,5,9-Triazacyclododecan-3-one, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

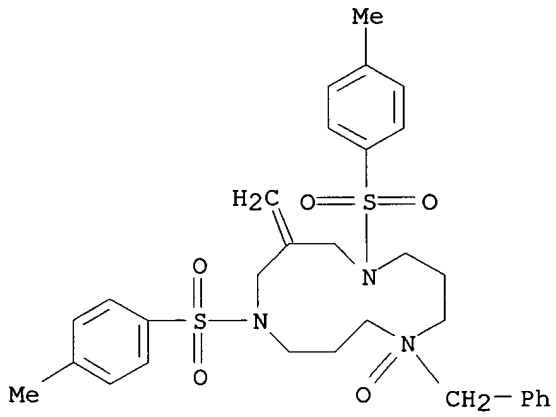


RN 182316-21-8 CAPLUS

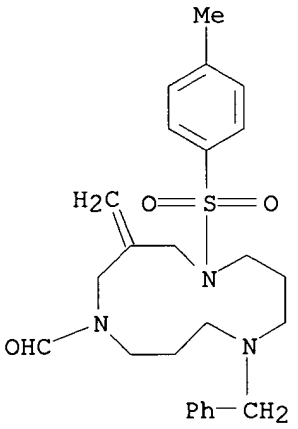
CN 1,5,9-Triazacyclododecane, 3-methyl-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



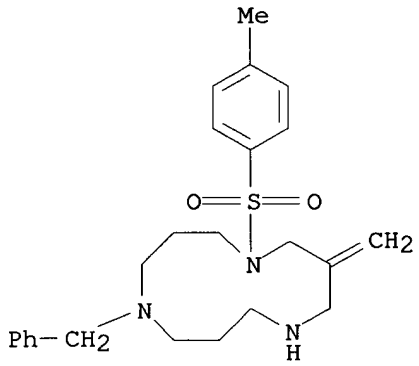
RN 182316-22-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)-, 9-oxide (9CI) (CA INDEX NAME)



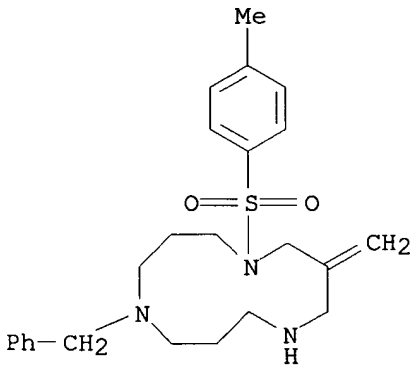
RN 182316-25-2 CAPLUS
CN 1,5,9-Triazacyclododecane-1-carboxaldehyde, 3-methylene-5-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



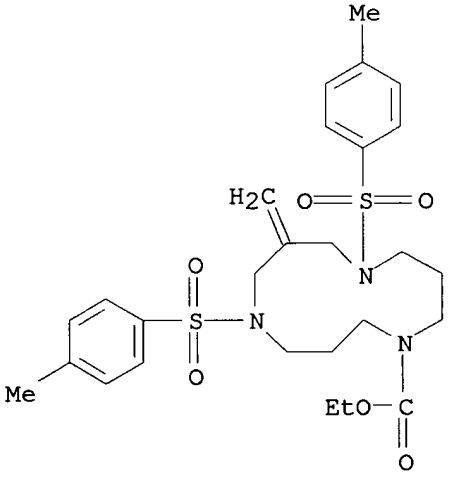
RN 182316-27-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



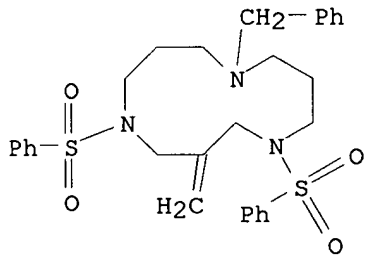
RN 182316-27-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



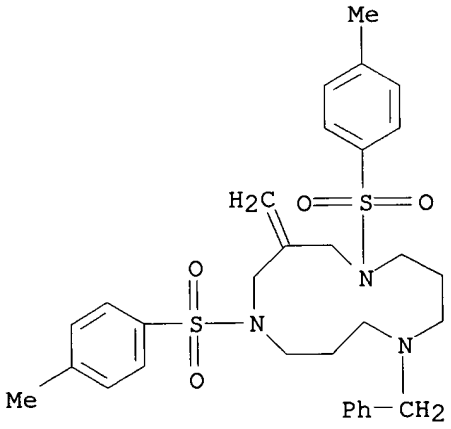
RN 182316-30-9 CAPLUS
CN 1,5,9-Triazacyclododecane-1-carboxylic acid, 7-methylene-5,9-bis[(4-methylphenyl)sulfonyl]-, ethyl ester (9CI) (CA INDEX NAME)



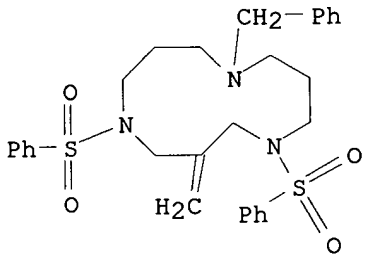
RN 182316-34-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-9-(phenylmethyl)-1,5-bis(phenylsulfonyl)- (9CI) (CA INDEX NAME)



RN 182316-44-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 182316-50-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-methylene-9-(phenylmethyl)-1,5-bis(phenylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)



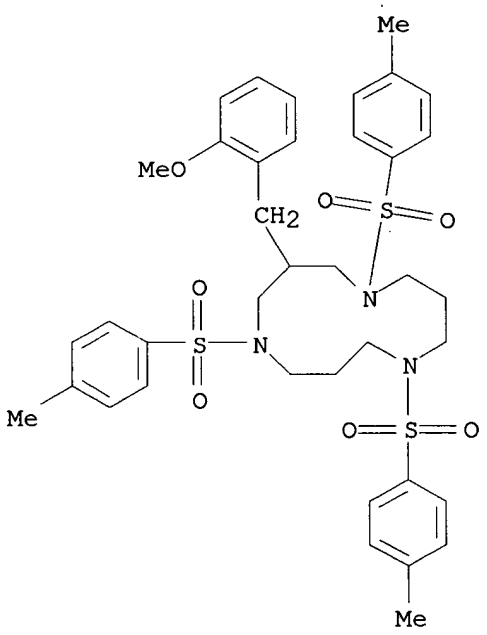
● HCl

L30 ANSWER 44 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:354980 CAPLUS
DOCUMENT NUMBER: 125:97175
TITLE: Complexation behavior of C- and N-functionalized tetradentate ligands based on 1,5,9-triazacyclododecane
AUTHOR(S): Bates, George B.; Parker, David
CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, DH1 3LE, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1996), (6), 1109-1115
CODEN: JCPKBH; ISSN: 0300-9580
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis and aqueous complexation behavior of C- and N-linked o-hydroxyaryl substituted derivs. of 1,5,9-triazacyclododecane is reported. The N-linked ligand forms strong 1:1 complexes with copper and zinc (log KML = 18.7 and 14.1, resp.) in which the phenolate acts as an effective donor ligand in the putative tetrahedral complex. The ligand substituted at carbon at the 3-position is less basic and forms much weaker complexes with Cu2+, Ni2+ and Zn2+ (log KCuL 10.2, log KZnL 7.32 and log KNiL 6.11) in which phenolate participation is absent.

IT 178879-52-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in preparation of hydroxybromobenzyl triazacyclododecane)

RN 178879-52-2 CAPLUS
CN 1,5,9-Triazacyclododecane, 3-[(2-methoxyphenyl)methyl]-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



L80 ANSWER 45 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:294877 CAPLUS
DOCUMENT NUMBER: 124:343341
TITLE: Preparation of cyclic polyamines as antiviral agents
INVENTOR(S): Iwata, Masaaki; Yamamoto, Naoki; Nakajima, Hideki
PATENT ASSIGNEE(S): Rikagaku Kenkyuzyo, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 35 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08027129	A2	19960130	JP 1994-165028	19940718
PRIORITY APPLN. INFO.:			JP 1994-165028	19940718

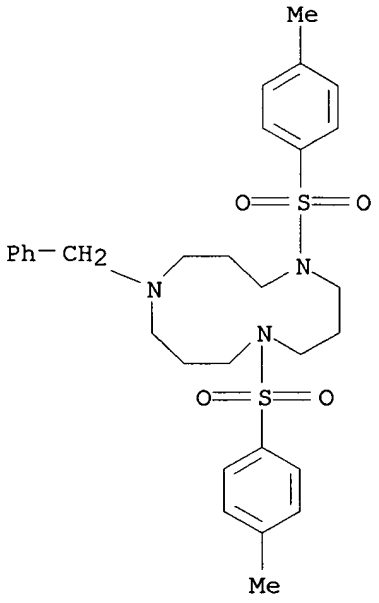
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

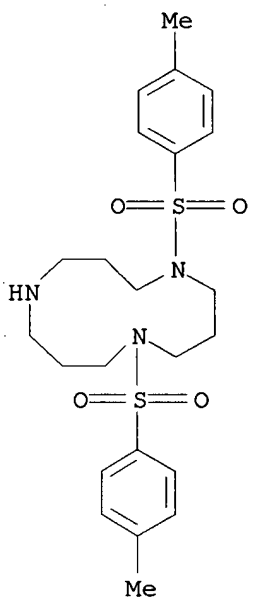
AB Cyclic polyazaalkanes, in which 3-20 C2, C3, or C4 alkylene chains and NH are alternately linked, are prepared Thus, the title compound (I.8HBr) was prepared by condensation of 1,5,9-triazacyclododecane derivative (III; Ts = p-toluenesulfonyl) with 1,3-dibromopropane in the presence of NaHCO3 at 70° for 4 days followed by detosylation. I.8HBr and another title compound (II.20HBr) showed ED50 of 2.5 and 0.67 μM for inhibiting the death of HIV-infected MT-4 cells (vs. 0.019 μM for AZT) and 50% cytotoxic concentration of 470 and 8.6 μM, resp., against MT-4 cells (vs. 247.25 μM).

IT 164913-15-9P 164913-31-9P 164913-40-0P
167080-92-4P 167080-93-5P 167080-99-1P
176493-19-9P 176493-21-3P 176493-22-4P
176493-23-5P 176493-25-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclic polyazaalkanes as antiviral agents)

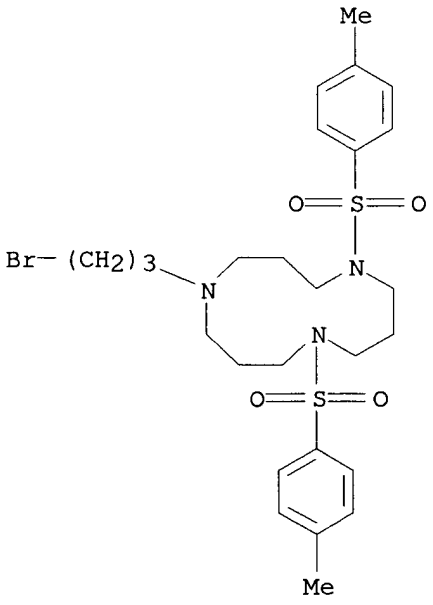
RN 164913-15-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 164913-31-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

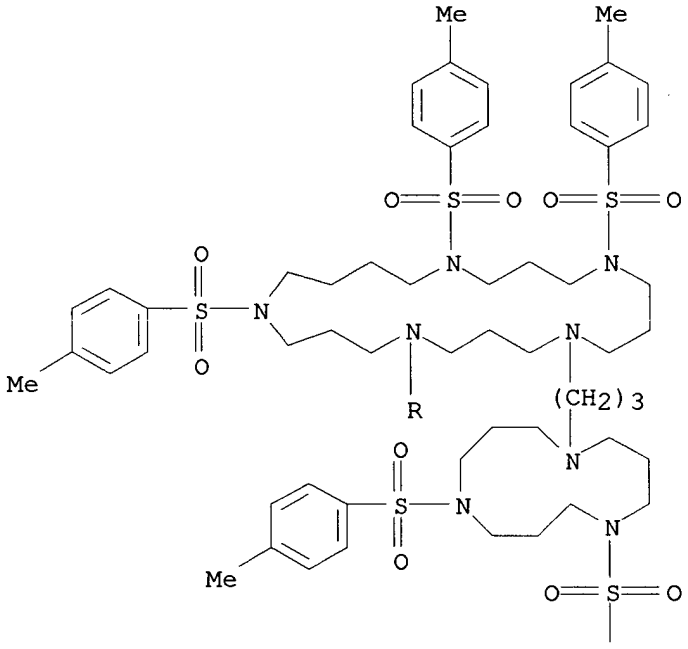


RN 164913-40-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 1-(3-bromopropyl)-5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

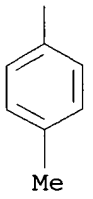


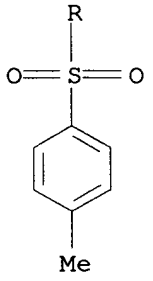
RN 167080-92-4 CAPLUS
CN 1,5,9,13,17-Pentaazacycloheneicosane, 9-[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,5,13,17-tetrakis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



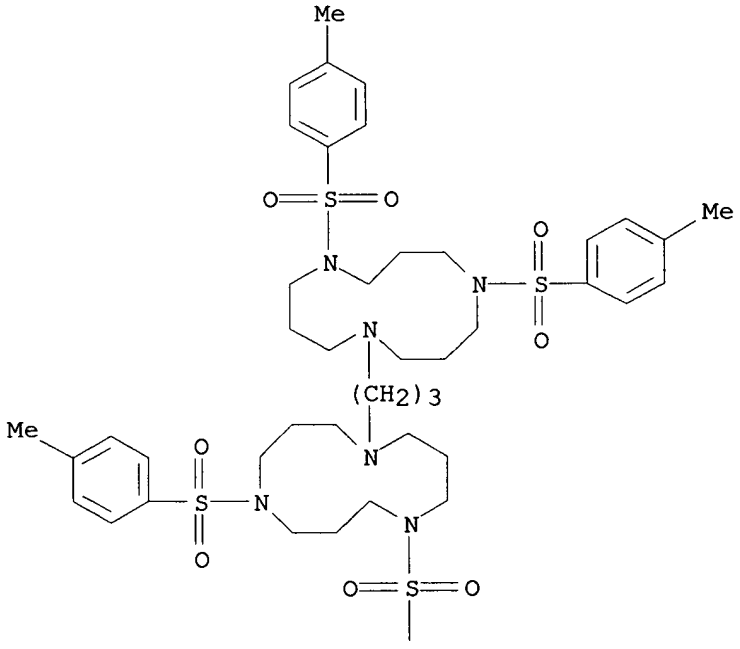
PAGE 2-A



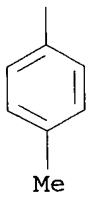


RN 167080-93-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,1'-(1,3-propanediyl)bis[5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

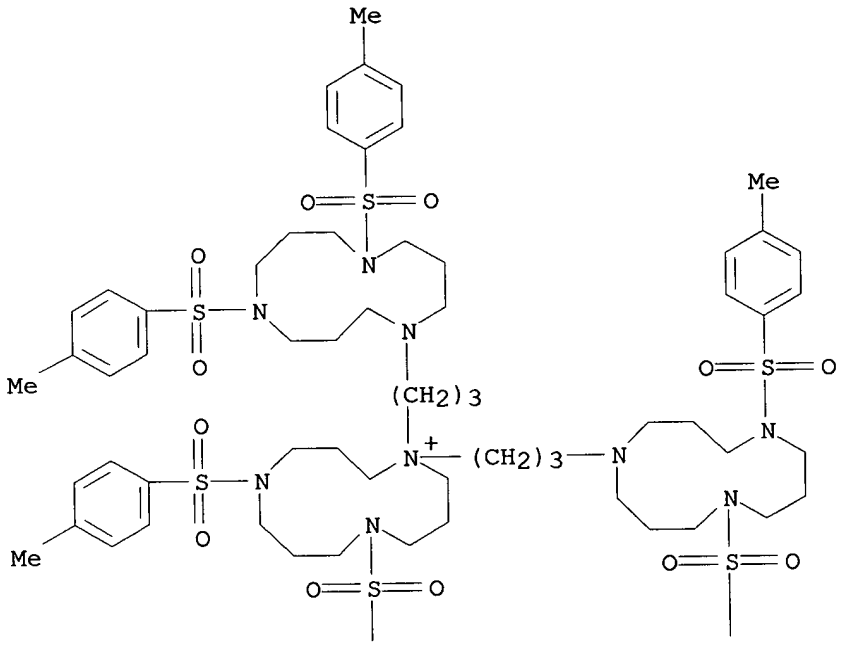


PAGE 2-A



RN 167080-99-1 CAPLUS
CN 5,9-Diaza-1-azoniacyclododecane, 1,1-bis[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-5,9-bis[(4-methylphenyl)sulfonyl]-, bromide (9CI) (CA INDEX NAME)

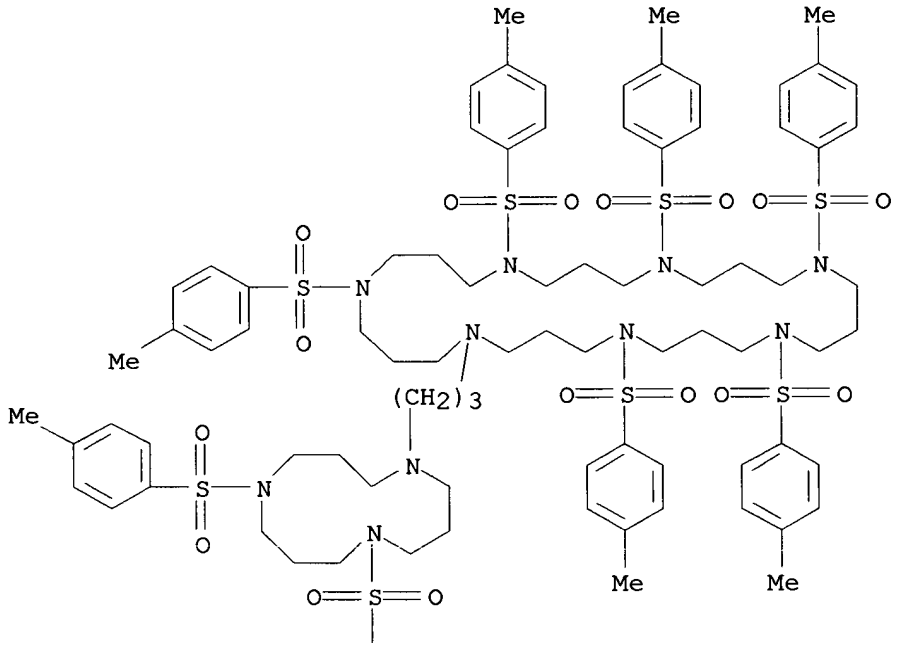
PAGE 1-A



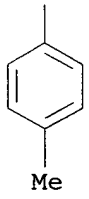
PAGE 2-A

RN 176493-19-9 CAPLUS
CN 1,5,9,13,17,21,25-Heptaazacyclooctacosane, 13-[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,5,9,17,21,25-hexakis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

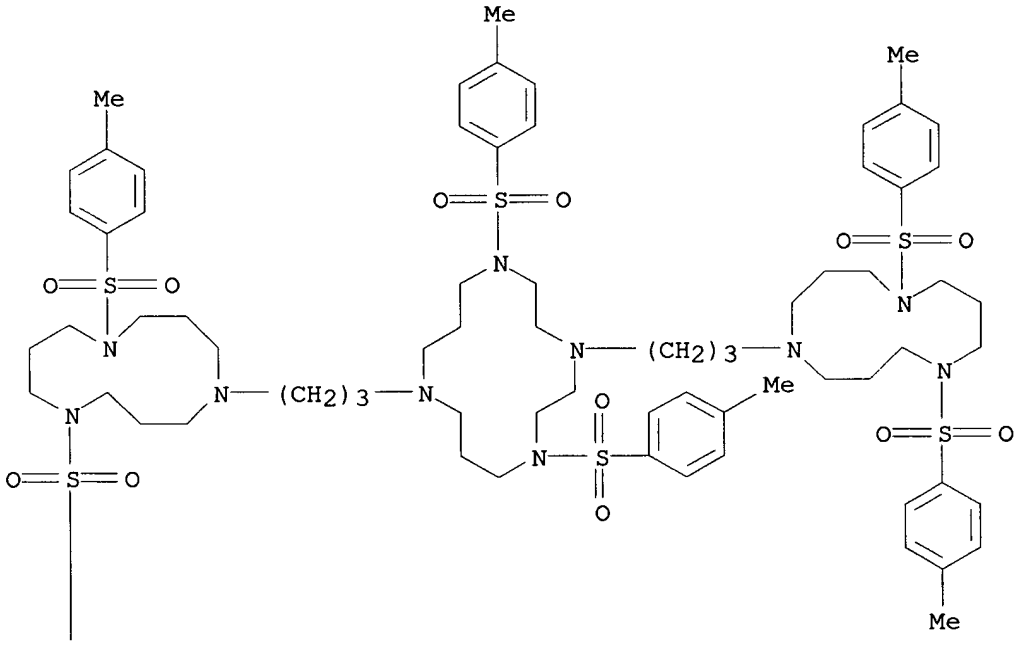


PAGE 2-A

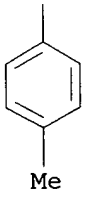


RN 176493-21-3 CAPLUS
CN 1,4,7,11-Tetraazacyclotetradecane, 4,11-bis[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,7-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



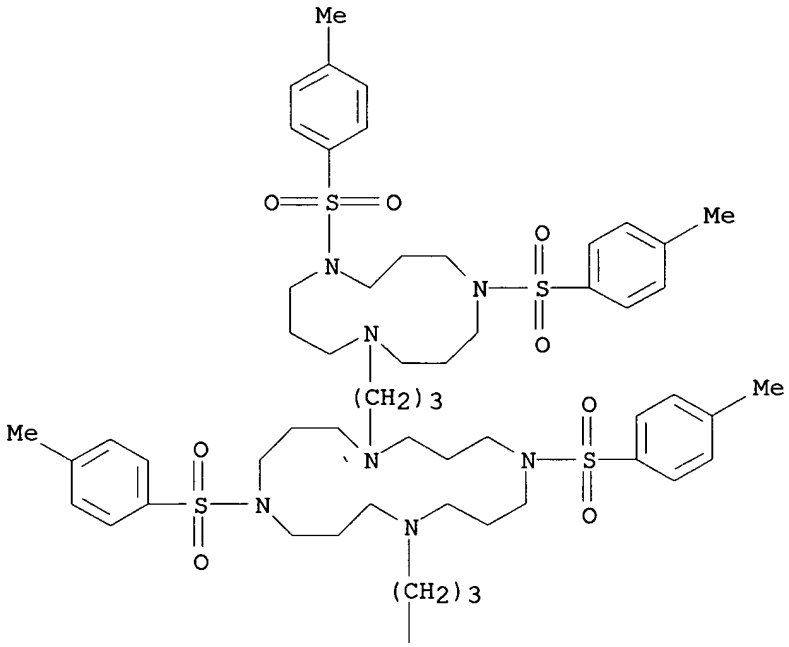
PAGE 2-A



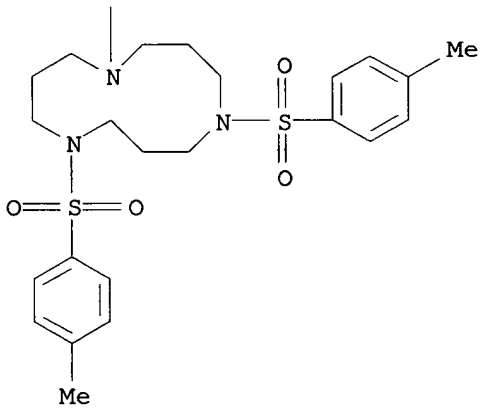
RN 176493-22-4 CAPLUS
CN 1,5,9,13-Tetraazacyclohexadecane, 1,9-bis[3-[5,9-bis[(4-

methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-5,13-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

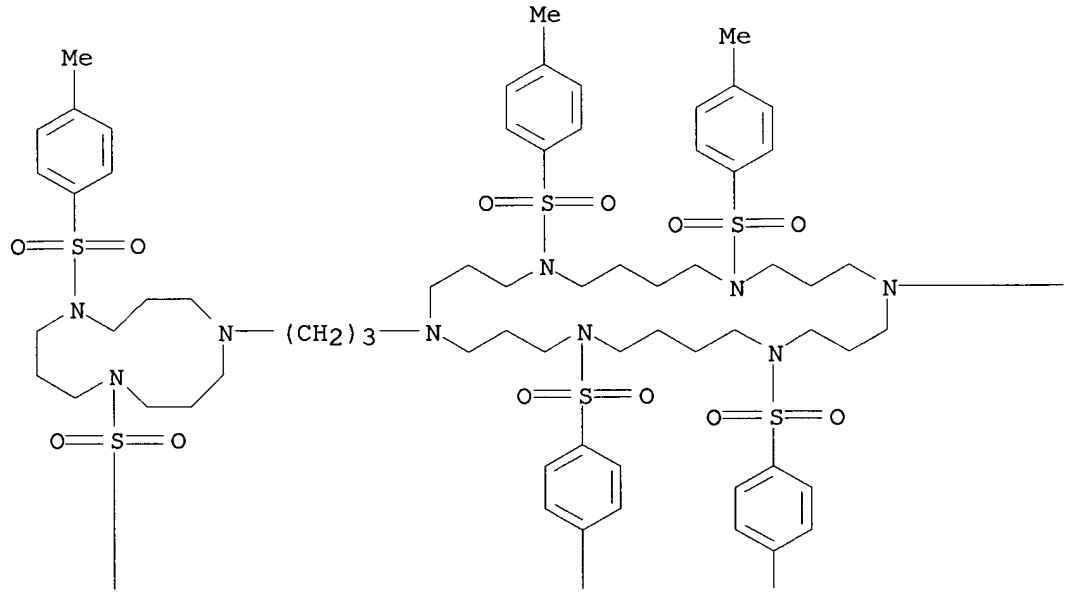


PAGE 2-A

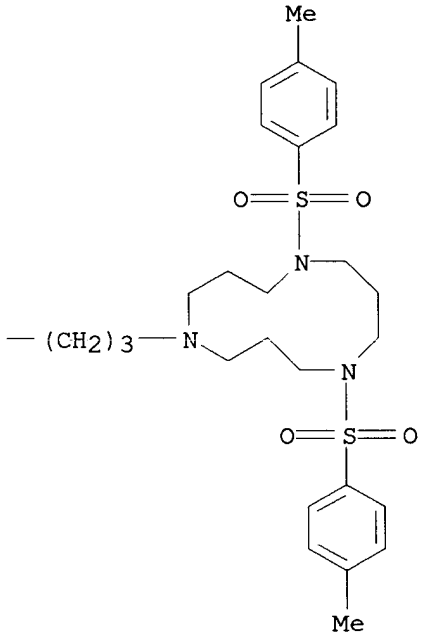


RN 176493-23-5 CAPLUS
CN 1,5,9,14,18,22-Hexaazacyclohexacosane, 5,18-bis[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,9,14,22-tetrakis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



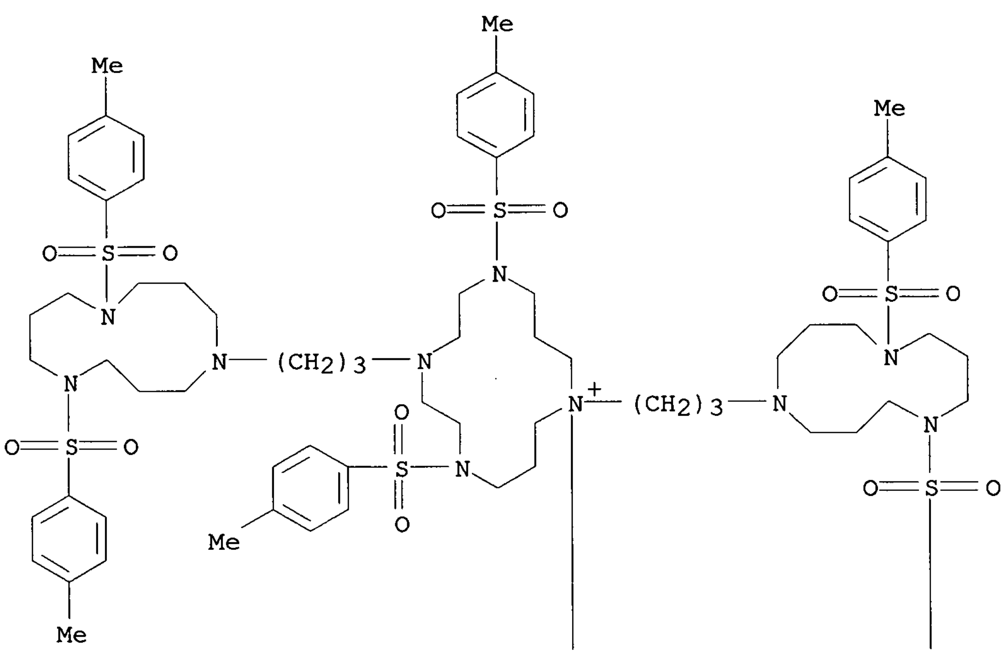
PAGE 1-B



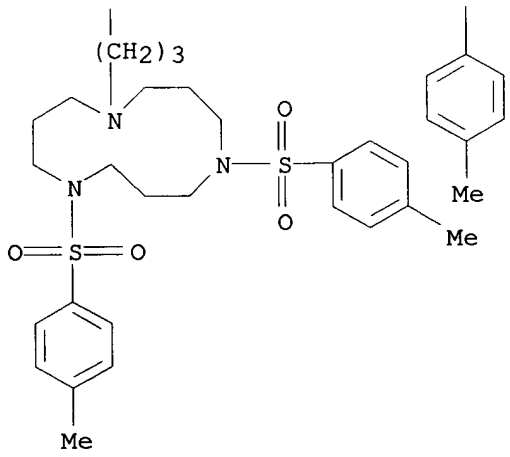
PAGE 2-A

RN 176493-25-7 CAPLUS
CN 1,4,7-Triaza-11-azoniacyclotetradecane, 4,11,11-tris[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,7-bis[(4-methylphenyl)sulfonyl]-, bromide (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



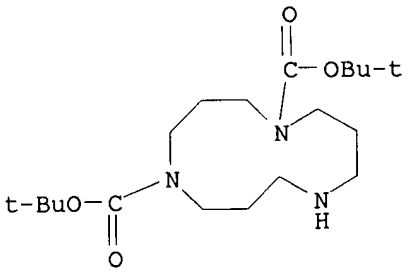
● Br^-

L30 ANSWER 46 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:157892 CAPLUS
DOCUMENT NUMBER: 124:305467
TITLE: New facile and convenient synthesis of bispolyazamacrocycles using Boc protection. Determination of geometric parameters of dinuclear copper(II) complexes using ESR spectroscopy and molecular mechanics calculations
AUTHOR(S): Brandes, Stephane; Gros, Claude; Denat, Franck; Pullumbi, Pluton; Guilard, Roger
CORPORATE SOURCE: Lab. d'Ingenierie Moleculaire Separation applications Gaz, Univ. Bourgogne, Dijon, 21100, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1996), 133(1), 65-73
CODEN: BSCFAS; ISSN: 0037-8968
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

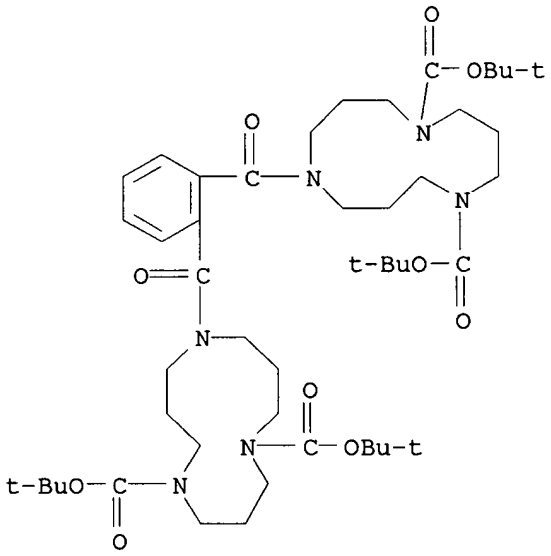
AB A new facile and convenient synthetic route was designed for the preparation of bispolyazamacrocycles in high yields by direct condensation of the readily available intermediate N,N'-diboctriazamacrocycle or N,N',N''-triboctetraazamacrocycles with aromatic biselectrophiles, ie, o-, m-, p-xylyl and anthracenyl derivs. The use of a versatile group, such as tert-butyloxycarbonyl (Boc), which is easily removed within 1 h by treatment with 6 M HCl or TFA, leads to polyazamacrocycles in which one N is discriminated from the others. The anthracenyl and o-xylyl dimers were synthesized by reacting diacyl chloride to give the corresponding diamides. Further reduction of the amide groups and elimination of the protecting Boc moieties were carried in a 1-pot reaction with BH3-THF followed by acid treatment. In parallel, exclusive mono-N-alkylation of the available secondary amine of the same protected macrocycle with the corresponding dibromoxylene gave the meta and para dimers; the protecting moieties were eliminated in a similar way. ESR measurements of spin-spin distances of the dicopper complexes were determined from the ratio of the intensity of the forbidden transition to the intensity of the allowed transitions. Mol. mechanics calcns. were also undertaken to evaluate the Cu-Cu distance by using a new rule-based force field.

IT 174192-40-6P 175854-44-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of bispolyazamacrocycles)

RN 174192-40-6 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 175854-44-1 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, 9,9'-(1,2-phenylenedicarbonyl)bis-, tetrakis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

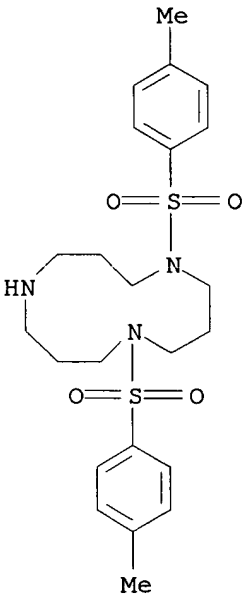


L30 ANSWER 47 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:113714 CAPLUS
DOCUMENT NUMBER: 124:202189
TITLE: Conversion of Macrocyclic Polyamines into Carbon-Substituted Derivatives. Synthesis of Derivatives of 1,5,9-Triazacyclododecane-2-carbonitrile
AUTHOR(S): Brunet, Philippe; Wuest, James D.
CORPORATE SOURCE: Departement de Chimie, Universite de Montreal, Montreal, QC, H3C 3J7, Can.
SOURCE: Journal of Organic Chemistry (1996), 61(5), 1847-9
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:202189

AB Diprotected derivs. of 1,5,9-triazacyclododecane were converted into diprotected derivs. of 1,5,9-triazacyclododecane-2-carbonitrile in good overall yield by oxidation with Na2WO4/H2O2, addition of KCN, and reduction with TiCl3. This strategy promises to be a useful general method for the direct conversion of macrocyclic polyamines into carbon-substituted derivs. that would otherwise not be readily available.

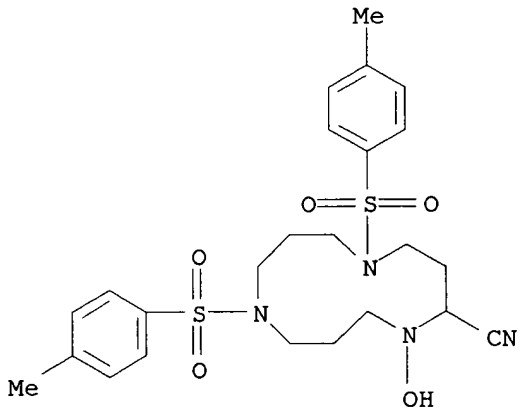
IT 164913-31-9P 174192-36-0P 174192-38-2P
174192-39-3P 174192-40-6P 174192-41-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(regioselective oxidative cyanation method for macrocyclic polyamines)

RN 164913-31-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

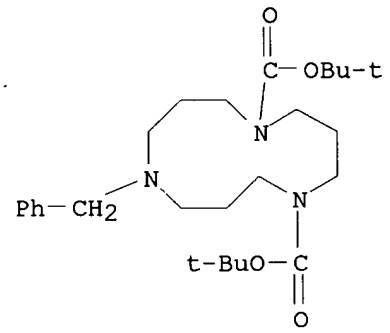


RN 174192-36-0 CAPLUS
CN 1,5,9-Triazacyclododecane-2-carbonitrile, 1-hydroxy-5,9-bis[(4-

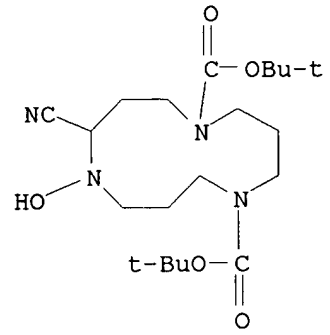
methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 174192-38-2 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, 9-(phenylmethyl)-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

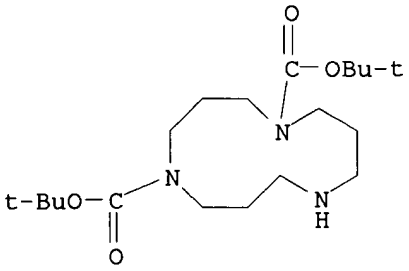


RN 174192-39-3 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, 8-cyano-9-hydroxy-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

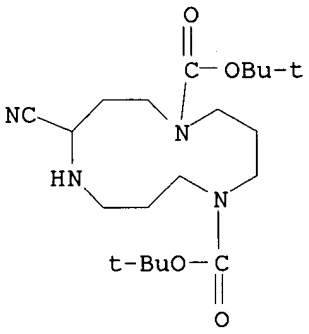


RN 174192-40-6 CAPLUS

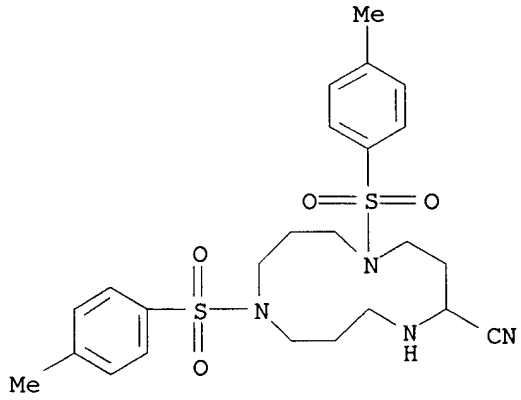
CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 174192-41-7 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-dicarboxylic acid, 8-cyano-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



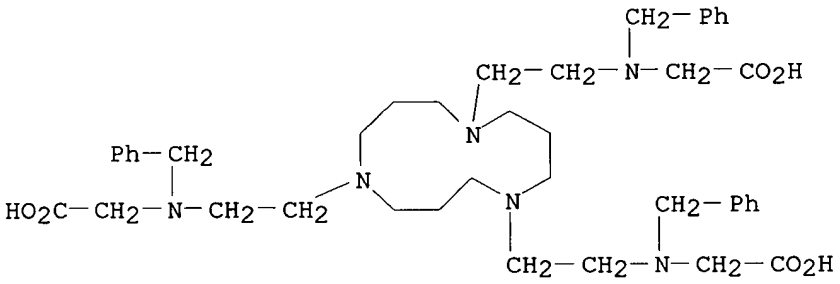
IT 174192-37-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective oxidative cyanation method for macrocyclic polyamines)
RN 174192-37-1 CAPLUS
CN 1,5,9-Triazacyclododecane-2-carbonitrile, 5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



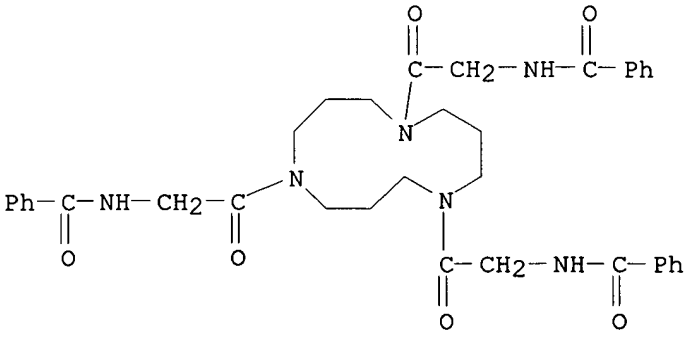
L30 ANSWER 48 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:77520 CAPLUS
DOCUMENT NUMBER: 124:232424
TITLE: Synthesis and characterization of a novel macrocyclic ligand containing nine donor atoms
AUTHOR(S): Giovenzana, G. B.; Jommi, G.; Pagliarin, R.; Sisti, M.; Aime, S.; Botta, M.; Geninatti, Crich, S.
CORPORATE SOURCE: Dip. Chim. Organica Industriale, Milan, I-20133, Italy
SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1996), 115(1), 94-8
CODEN: RTCPA3; ISSN: 0165-0513
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis of a novel macrocyclic ligand containing nine potential coordination sites (six nitrogens and three oxygens) formed by a triazacyclododecane ring trisubstituted with -CH2-CH2-N(CH2Ph)-CH2COOH groups is reported. The protonation scheme of this ligand has been elucidated by measuring the proton NMR shifts of the various methylenic resonances upon changing the pH of the solution This ligand affords stable metal complexes with Cd2+ ion, whose 1H- and 13C-NMR spectra suggest a remarkable kinetic inertia and stereochem. rigidity.

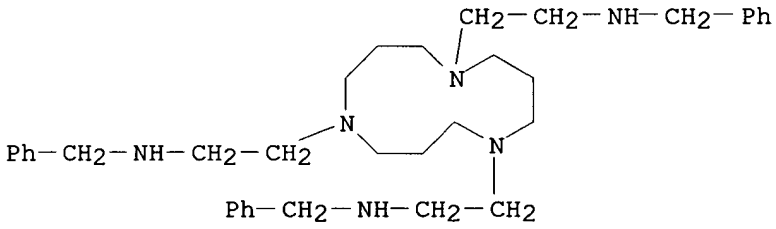
IT 174783-36-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 174783-36-9 CAPLUS
CN Glycine, N,N',N''-(1,5,9-triazacyclododecane-1,5,9-triyltri-2,1-ethanediyl)tris[N-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT 174783-34-7P 174783-35-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and characterization of a novel macrocyclic ligand containing nine donor atoms)
RN 174783-34-7 CAPLUS
CN Benzamide, N,N',N''-[1,5,9-triazacyclododecane-1,5,9-triyltris(2-oxo-2,1-ethanediyl)]tris- (9CI) (CA INDEX NAME)



RN 174783-35-8 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triethanamine, N,N',N''-tris(phenylmethyl)- (9CI) (CA INDEX NAME)

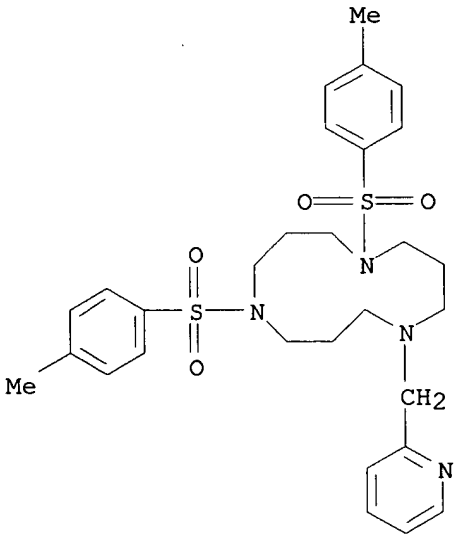


L30 ANSWER 49 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:953685 CAPLUS
DOCUMENT NUMBER: 124:74712
TITLE: Synthesis and coordination chemistry of the pyridyl pendant-arm azamacrocycles 1-(2-pyridylmethyl)-1,5,9-triazacyclododecane L1 and 1-(2-pyridyl-2'-ethyl)-1,5,9-triazacyclododecane L2, with nickel(II), copper(II) and zinc(II). Crystal structures of [Ni(L1)(O2NO)]NO3 and [ZnL2][Zn(NO3)3.67Cl0.33]
AUTHOR(S): Turonek, Mary L.; Moore, Peter; Clase, Howard J.; Alcock, Nathaniel W.
CORPORATE SOURCE: Dep. Chem., University of Warwick, Coventry, CV4 7AL, UK
SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1995), (22), 3659-66
CODEN: JCDTBI; ISSN: 0300-9246
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

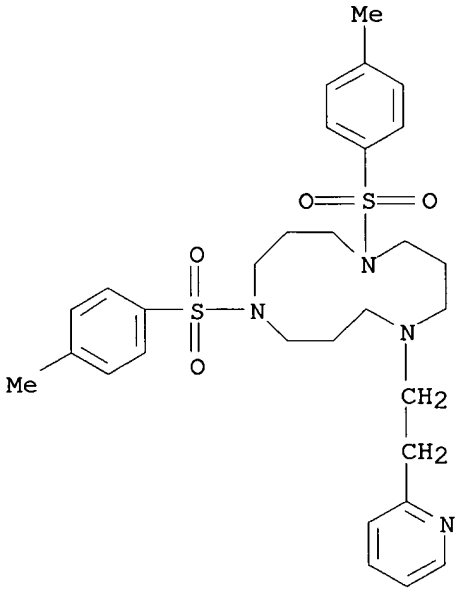
AB The azamacrocyclic ligands 1-(2-pyridylmethyl)-1,5,9-triazacyclododecane L1 and 1-(2-pyridyl-2'-ethyl)-1,5,9-triazacyclododecane L2 were prepared, and their complexes with hydrated Ni(II), Cu(II) and Zn(II) nitrates were isolated. The Ni(II) complexes are high spin and six-coordinate, while 13C NMR spectroscopy shows that [ZnL1(OH)2]2+ exists as a sym. trigonal bipyramidal isomer in solution, and [ZnL2]2+ exists as a 2:1 mixture of tetrahedral and asym. trigonal-bipyramidal isomers. X-ray crystallog. was used to determine the solid-state structures of the octahedral [NiL1(O2NO)]+, and the tetrahedral isomer of [ZnL2]2+.

IT 172101-45-0P, 1-(2-Pyridylmethyl)-5,9-bis(toluene-p-sulfonyl)-1,5,9-triazacyclododecane 172101-50-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of pyridylalkyltriazacyclododecane)

RN 172101-45-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



RN 172101-50-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-[2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



L80 ANSWER 50 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:763501 CAPLUS
DOCUMENT NUMBER: 123:169670
TITLE: Preparation of macrocyclic polyamine derivatives
INVENTOR(S): Iwata, Masaaki
PATENT ASSIGNEE(S): Rikagaku Kenkyuzyo, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 58 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06256512	A2	19940913	JP 1993-71147	19930305
PRIORITY APPLN. INFO.:			JP 1993-71147	19930305

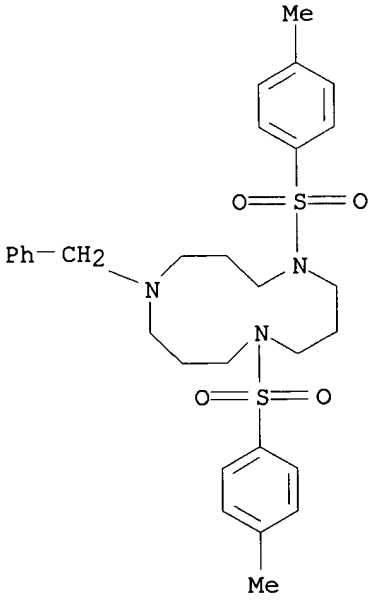
OTHER SOURCE(S): MARPAT 123:169670
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

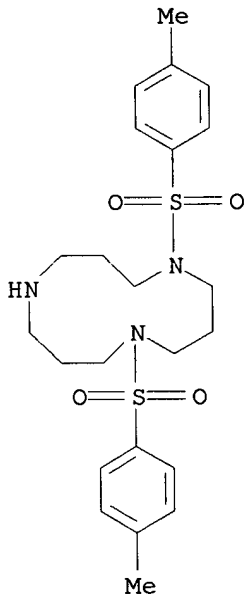
AB Macrocyclic polyamines e.g. compds. I (Ts = tosyl) and II (R = Ts, H) and their salts, having biomimetic functions and useful as catalysts (no data), were prepared Thus,stirring N5,N9,N17,N21-tetratosyl-1,5,9,13,17,21-hexaazacyclotetracosane with N1-(3-bromopropyl)-N5,N9-ditosyl-1,5,9-triazacyclododecane and NaHCO3 in MeCN at room temperature for 2 days gave 82% I.

IT 164913-15-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of macrocyclic polyamine derivs.)

RN 164913-15-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

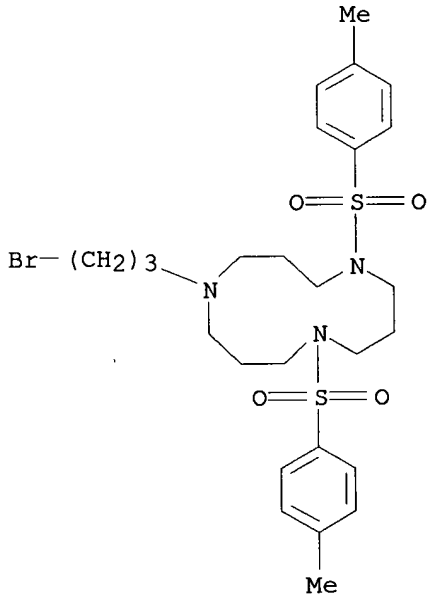


IT 164913-31-9P 164913-40-0P 167080-90-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of macrocyclic polyamine derivs.)
RN 164913-31-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



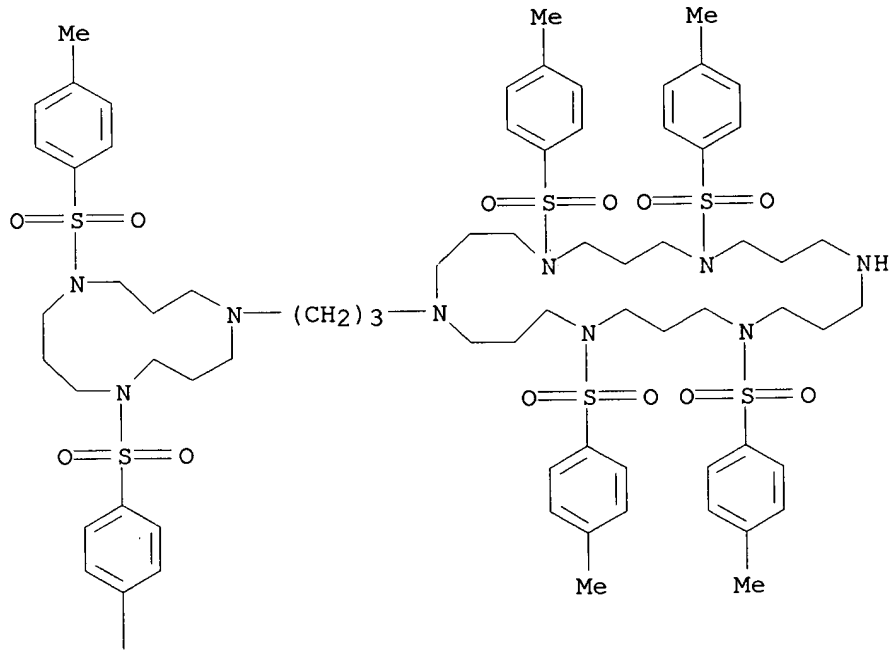
RN 164913-40-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 1-(3-bromopropyl)-5,9-bis[(4-

methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 167080-90-2 CAPLUS
CN 1,5,9,13,17,21-Hexaazacyclotetracosane, 9-[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,5,13,17-tetrakis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

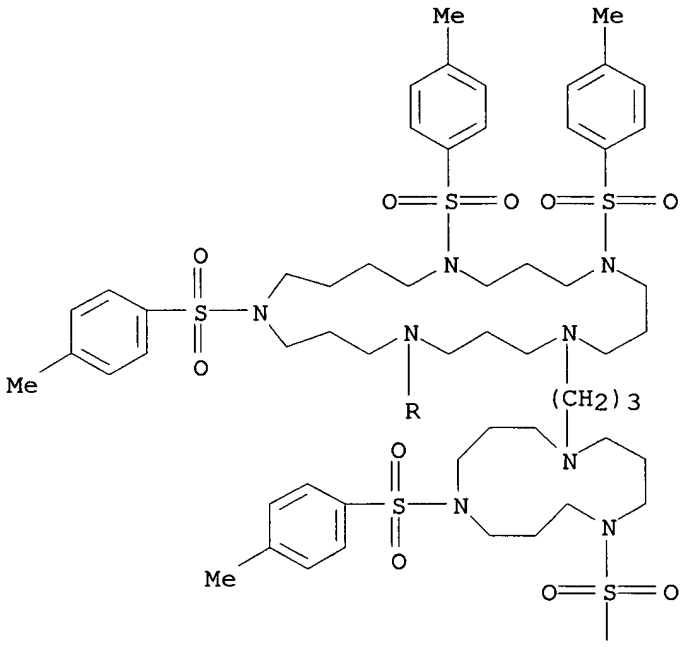


PAGE 2-A

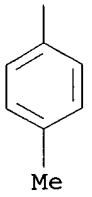
Me

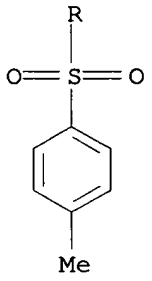
IT 167080-92-4P 167080-93-5P 167080-94-6P
167080-97-9P 167080-99-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of macrocyclic polyamine derivs.)
RN 167080-92-4 CAPLUS
CN 1,5,9,13,17-Pentaazacycloheneicosane, 9-[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,5,13,17-tetrakis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



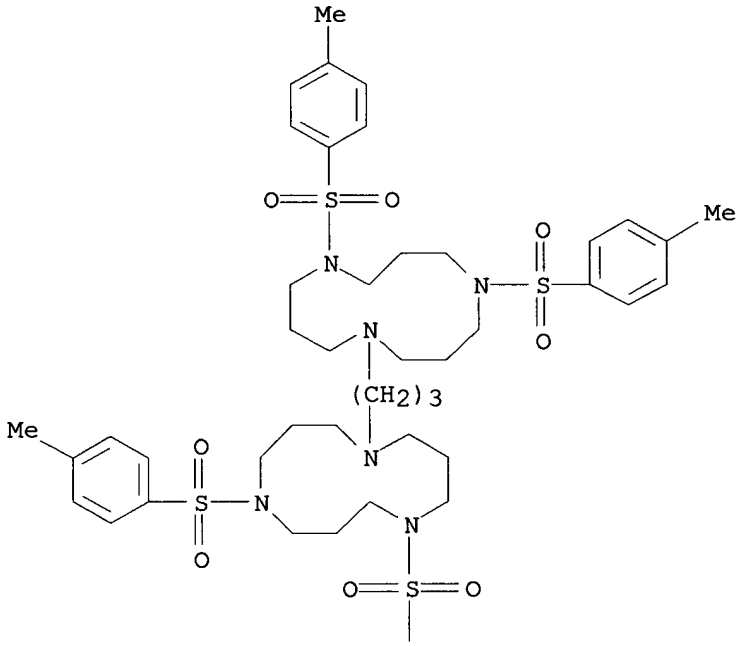
PAGE 2-A



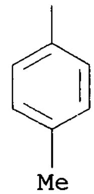


RN 167080-93-5 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,1'-(1,3-propanediyl)bis[5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

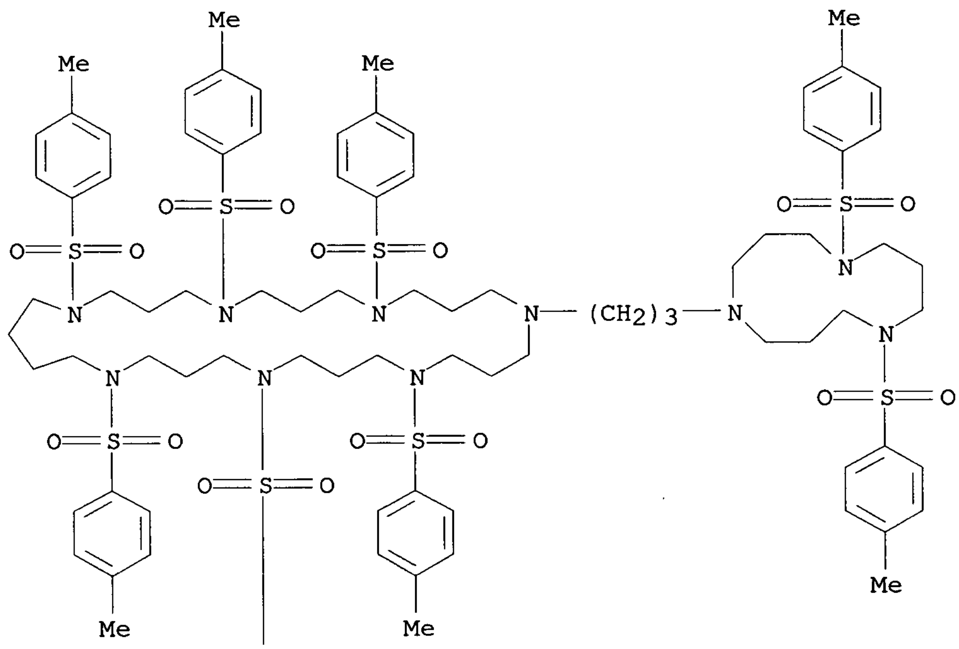


PAGE 2-A

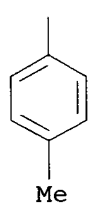


RN 167080-94-6 CAPLUS
CN 1,5,9,13,17,21,25-Heptaazacyclononacosane, 13-[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-1,5,9,17,21,25-hexakis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



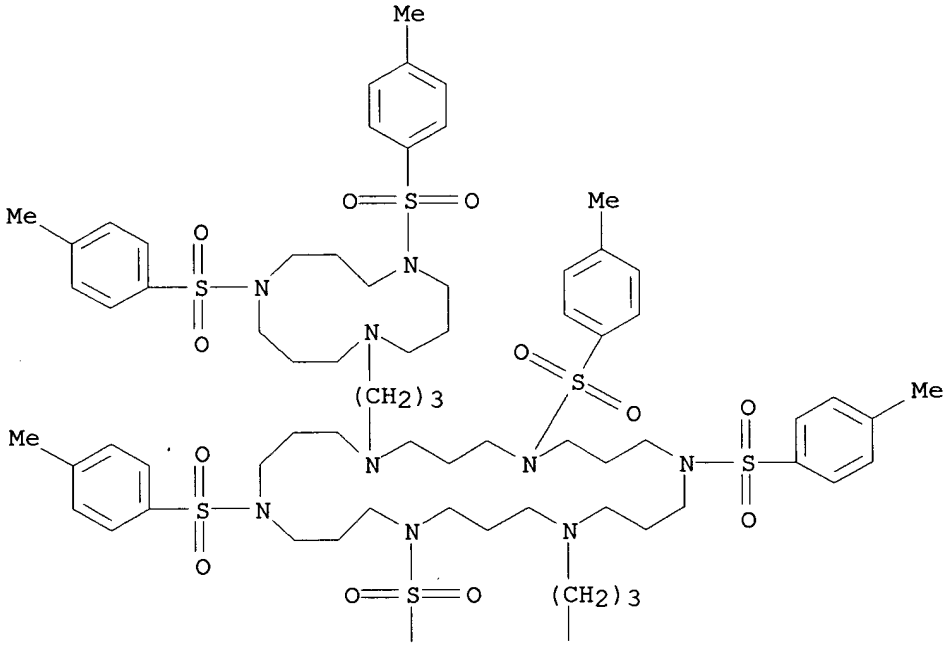
PAGE 2-A



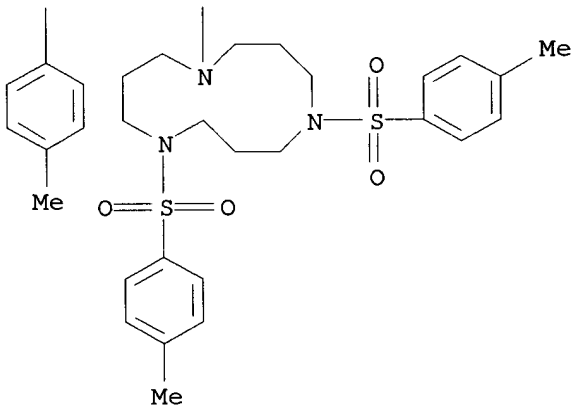
RN 167080-97-9 CAPLUS
CN 1,5,9,13,17,21-Hexaazacyclotetracosane, 1,13-bis[3-[1,5-bis[(4-

methylphenyl)sulfonyl]-1,5,9-triazacyclododec-9-yl]propyl]-5,9,17,21-tetrakis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

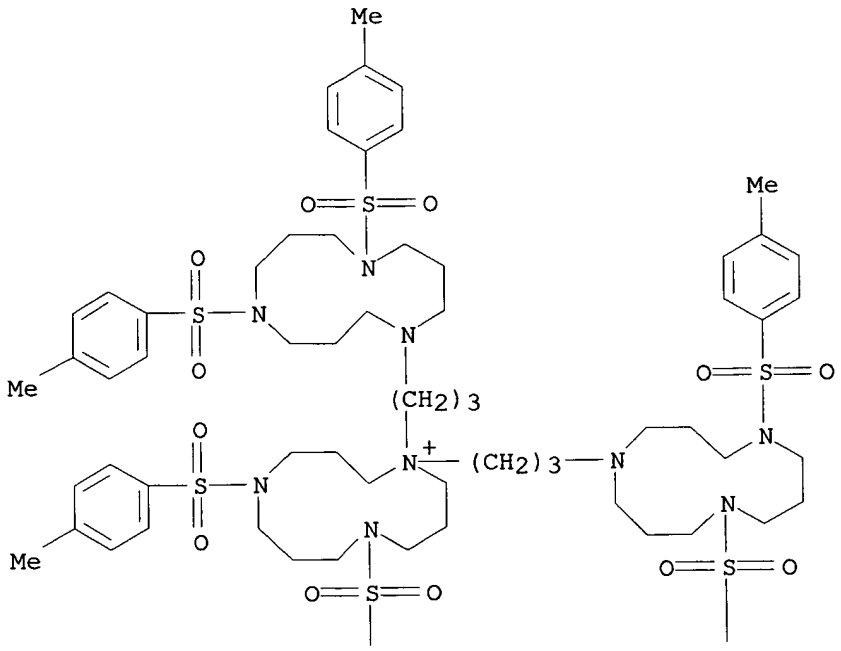


PAGE 2-A

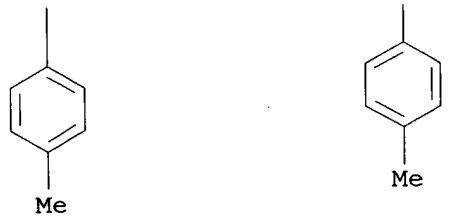


RN 167080-99-1 CAPLUS
CN 5,9-Diaza-1-azoniacyclododecane, 1,1-bis[3-[5,9-bis[(4-methylphenyl)sulfonyl]-1,5,9-triazacyclododec-1-yl]propyl]-5,9-bis[(4-methylphenyl)sulfonyl]-, bromide (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

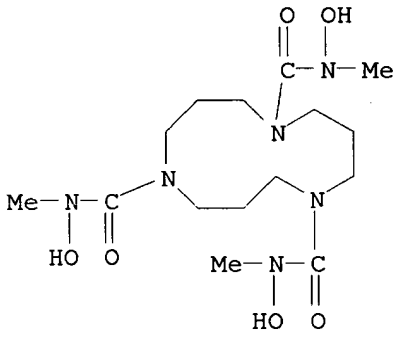


L90 ANSWER 51 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:740701 CAPLUS
DOCUMENT NUMBER: 123:267802
TITLE: Siderophore analogs. Synthesis and chelating properties of a new macrocyclic trishydroxamate ligand
AUTHOR(S): Esteves, M. Alexandra; Vaz, M. Candida T.; Goncalves, M. L. S. Simoes; Farkas, Etelka; Santos, M. Amelia
CORPORATE SOURCE: Cent. Quim. Estrutural, Inst. Superior Tecnico, Lisbon, 1096, Port.
SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1995), (15), 2565-73
CODEN: JCDTBI; ISSN: 0300-9246
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new Fe(III)-specific ligand, 1,5,9-triazacyclododecane-N,N',N''-tris(N-methylacetohydroxamic acid) H3L, containing three hydroxamic acid groups as pendant arms on a macrocyclic triamine backbone, was synthesized and characterized. Its acid-base and chelating properties with Fe(III) and Cu(II) ions were studied by potentiometric and spectrophotometric techniques. The mechanism of electron transfer as well as the kinetics of dissociation and stability consts. of reduced species, which probably are important in the biol. activity of this siderophore analog, were studied by voltammetric methods. This ligand proved to be biol. active and its properties were compared with ferrichrome and ferrioxamine B.

IT 169386-06-5
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(synthesis and complexation of new macrocyclic trishydroxamate ligand with iron(3+) and copper(2+))

RN 169386-06-5 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tricarboxamide, N,N',N''-trihydroxy-N,N',N''-trimethyl- (9CI) (CA INDEX NAME)



L30 ANSWER 52 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:677172 CAPLUS
DOCUMENT NUMBER: 123:55936
TITLE: Preparation of intermediates of macrocyclic polyamines
INVENTOR(S): Iwata, Masaaki
PATENT ASSIGNEE(S): Rikagaku Kenkyuzyo, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 29 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

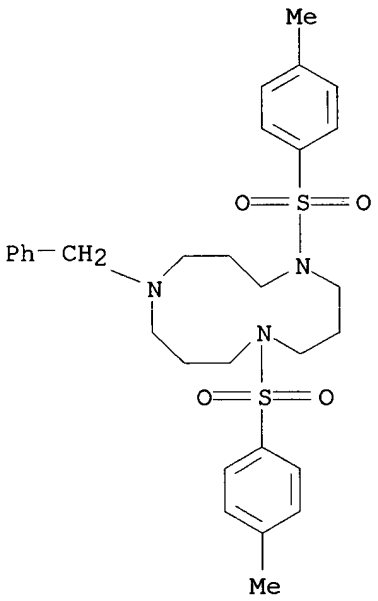
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06211776	A2	19940802	JP 1993-23663	19930119

PRIORITY APPLN. INFO.: JP 1993-23663 19930119
OTHER SOURCE(S): MARPAT 123:55936

AB Title intermediates e.g. N8-benzyl-N1,N4,N12,N15-tetratosyl-4,8,12-triaza-1,15-pentadecanediamine, O1,O12-dimesyl-N4,N9-ditosyl-4,9-diaza-1,12-dodecanediol, N,N-bis(3-bromopropyl)benzylamine (I), and N5,N10,N14,N18,N22,N27-hexatosyl-1,5,10,14,18,22,27-heptaazacyclotriacontane were prepared Thus, stirring benzylamine with 1,3-dibromopropane and NaHCO3 in MeCN at 60° for 22 h gave 37% I.

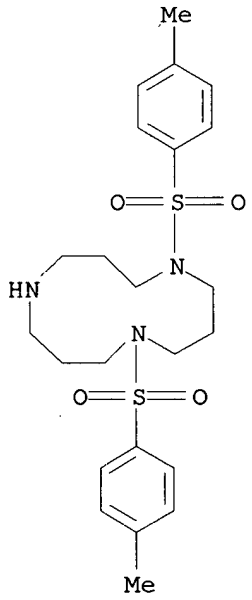
IT 164913-15-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of intermediates of macrocyclic polyamines)

RN 164913-15-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

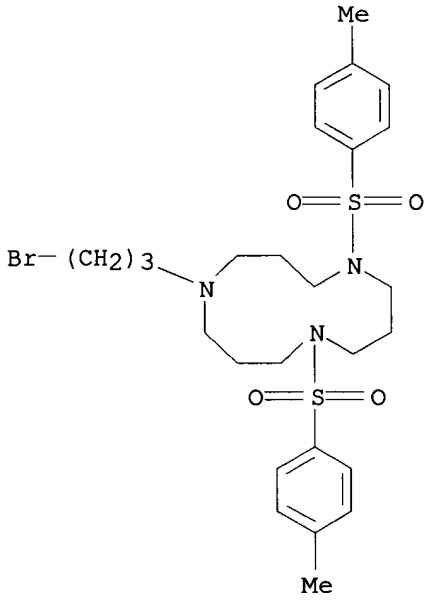


IT 164913-31-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of intermediates of macrocyclic polyamines)
RN 164913-31-9 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



IT 164913-40-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of intermediates of macrocyclic polyamines)
RN 164913-40-0 CAPLUS
CN 1,5,9-Triazacyclododecane, 1-(3-bromopropyl)-5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

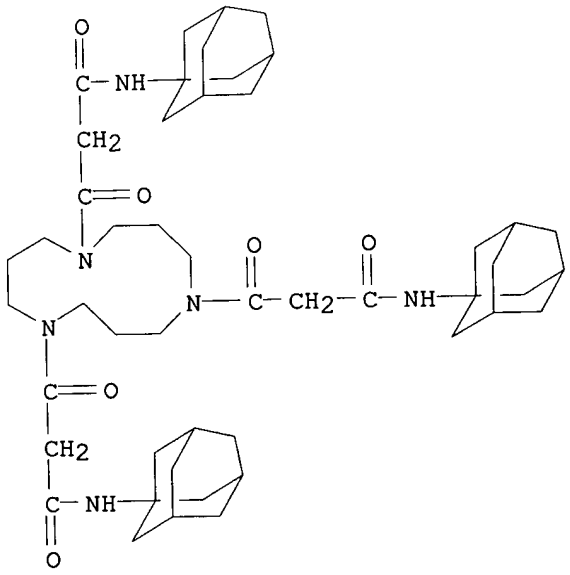

Me
O
S
O
Br
(CH2)3
N
N
N
O
S
O
Me

L30 ANSWER 53 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:283587 CAPLUS
DOCUMENT NUMBER: 122:229436
TITLE: Design and Synthesis of Calcium and Magnesium Ionophores Based on Double-Armed Diazacrown Ether Compounds and Their Application to an Ion Sensing Component for an Ion-Selective Electrode
AUTHOR(S): Suzuki, Koji; Watanabe, Kazuhiko; Matsumoto, Yukihiro; Kobayashi, Mitsuru; Sato, Sayaka; Siswanta, Dwi; Hisamoto, Hideaki
CORPORATE SOURCE: Department of Applied Chemistry, Keio University, Yokohama, 223, Japan
SOURCE: Analytical Chemistry (1995), 67(2), 324-34
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The double-armed diazacrown ethers, which have a base diazacrown ether ring with two diamide-type side chains, were designed and synthesized from the proposed mol. model for the novel neutral Ca2+ and Mg2+ ionophores. The potentiometric ion-selective electrodes were prepared with over 20 kinds of systematically synthesized diazacrown ether derivs. The relation between the mol. structures of the ionophores and the ion selectivities was fully discussed. The electrodes based on the 21- and 18-membered diazacrown ether derivs. possessing a glycolic diamide and malonic diamide in their side chains (K23E1 and K22B5) exhibited excellent Ca2+ and Mg2+ selectivities, resp. The ion-selectivity features of the novel Ca2+ and Mg2+ ionophores supply important structural information about the design of host mols. for alkaline earth metal cations.

IT 162008-35-7P, 1,5,9-Tris[(N-(1-adamantyl)carbamoyl)acetyl]-1,5,9-triazacyclododecane
RL: ARU (Analytical role, unclassified); DEV (Device component use); PNU (Preparation, unclassified); PRP (Properties); ANST (Analytical study); PREP (Preparation); USES (Uses)
(design and synthesis of calcium and magnesium ionophores based on double-armed diazacrown ether compds. and application to ion sensing component for ion-selective electrode)

RN 162008-35-7 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-tripropanamide, β,β',β''-trioxo-N,N',N''-tris(tricyclo[3.3.1.13,7]dec-1-yl)- (9CI) (CA INDEX NAME)

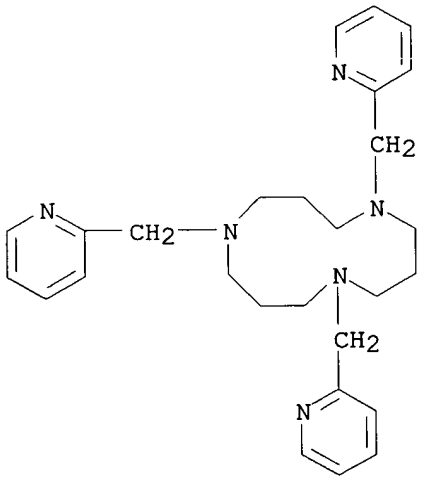


L30 ANSWER 54 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:64905 CAPLUS
DOCUMENT NUMBER: 122:44835
TITLE: Synthesis, Characterization, and Molecular Mechanics Studies on the Metal Complexes of 1,5,9-Tris(2-pyridylmethyl)-1,5,9-triazacyclododecane, [ML1](PF6)2 (M = Fe(II), Mn(II), Co(II), Ni(II), Cu(II), Pd(II))
AUTHOR(S): Zhang, Delong; Busch, Daryle H.
CORPORATE SOURCE: Department of Chemistry, University of Kansas, Lawrence, KS, 66045, USA
SOURCE: Inorganic Chemistry (1994), 33(22), 5138-43
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

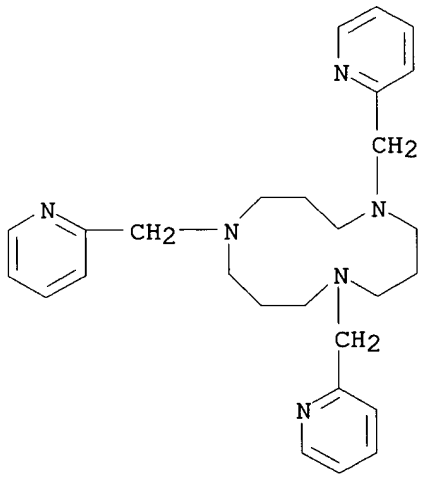
AB 1,5,9-Tris(2-pyridylmethyl)-1,5,9-triazacyclododecane (L1) and [ML1](PF6)2 (M = Fe(II), Mn(II), Co(II), Ni(II), Cu(II), Pd(II)), were prepared and characterized. The effective magnetic moments at room temperature are 5.68, 6.004.38, 3.23, and 2.10 μB, resp., for the Fe(II), Mn(II), Co(II), Ni(II), and Cu(II) complexes, and Pd(II) complex is diamagnetic. Cyclic voltammetry provided the potentials for the quasireversible redox couples Fe(III)/Fe(II) and Mn(III)/Mn(II) and for the reversible couples Cu(II)/Cu(I) and Pd(II)/Pd(I): 1.22, 1.48, -0.21, and -0.77 V, resp. [CoIIL1]2+, [NiIIL1]2+, and [PdIIL1]2+ are irreversibly oxidized at 1.49, 1.9, and 1.27 V vs. normal H electrode. The new complexes are much more resistant to oxidation than the analogous derivs. of 1,4,7-tris(2-pyridylmethyl)-1,4,7-triazacyclononane. This difference in behavior is rationalized from mol. mechanics calcns. that show the min. strain energy M-N(sp3) distances to be 2.37 Å for a1,5,9-tris(2-pyridylmethyl)-1,5,9-triazacyclododecane complex and 2.12 Å for a 1,4,7-tris(2-pyridylmethyl)-1,4,7-triazacyclononane complex. The influence of the triaza ring size on the phys. properties of the complexes is also discussed.

IT 102851-51-4, 1,5,9-Tris(2-pyridylmethyl)-1,5,9-triazacyclododecane
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of transition metal homoleptic complexes)

RN 102851-51-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



IT 102851-51-4DP, palladium complex
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and cyclic voltammetry and mol. mech. calcns. for coordinate bond strain energy of)
RN 102851-51-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



L80 ANSWER 55 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:534168 CAPLUS
DOCUMENT NUMBER: 121:134168
TITLE: Preparation of N-substituted-polyazamacrocycles as chelants
INVENTOR(S): Sherry, A. Dean; Van Westrenen, Jeroen
PATENT ASSIGNEE(S): Board of Regents, the University of Texas System, USA
SOURCE: U.S., 40 pp. Cont.-in-part of U.S. Ser. No. 615,619.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5316757	A	19940531	US 1991-808845	19911213
US 4639365	A	19870127	US 1984-662075	19841018
US 4983376	A	19910108	US 1988-291053	19881228
US 5342606	A	19940830	US 1990-615619	19901119
WO 9312097	A1	19930624	WO 1992-US9247	19921027
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9229124	A1	19930719	AU 1992-29124	19921027
AU 659244	B2	19950511		
EP 618910	A1	19941012	EP 1992-923096	19921027
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, SE				
ZA 9208338	A	19930504	ZA 1992-8338	19921028
CN 1073680	A	19930630	CN 1992-114146	19921211
CN 1033803	B	19970115		
US 5428155	A	19950627	US 1994-250048	19940527

PRIORITY APPLN. INFO.:

US 1984-662075	A2	19841018
US 1987-7729	A2	19870127
US 1988-291053	A2	19881228
US 1989-357193	B2	19890525
US 1990-615619	A2	19901119
US 1991-808845	A	19911213
WO 1992-US9247	A	19921027

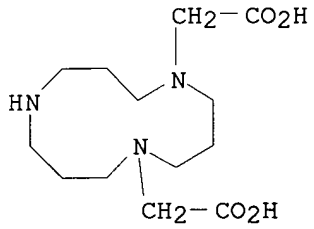
OTHER SOURCE(S): MARPAT 121:134168

AB Title compds. [e.g., 1,4,7,10-tetraazacyclododecane(N,N''-diacetic acid)(N'R1)(N'''R2); R1,R2 = H, CH2CH2OH, CH2CHMeOH, CH2P(O)Et(O-), CH2P(O)(OEt)(O-), CH2PO32-] were prepared as chelants for MRI contrast agents and NMR shift reagents (no data). Thus, 1,4,7,10-tetraazacyclododecane was heated at 40° for 16h in aqueous solution with HCHO.Na2SO3 and the product treated with NaCN to give, after HCl hydrolysis, 1,4,7,10-tetraazacyclododecane-N,N''-diacetic acid hydrochloride.

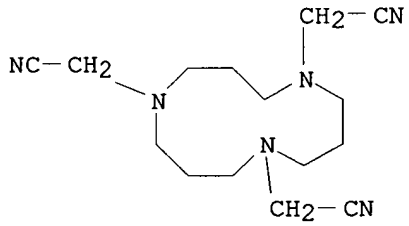
IT 127603-37-6P 144003-25-8P 157282-08-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, in preparation of chelant)

RN 127603-37-6 CAPLUS

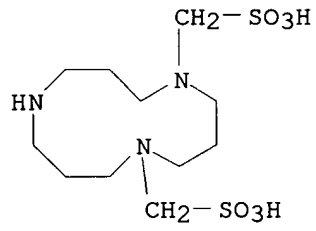
CN 1,5,9-Triazacyclododecane-1,5-diacetic acid (9CI) (CA INDEX NAME)



RN 144003-25-8 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triacetonitrile (9CI) (CA INDEX NAME)



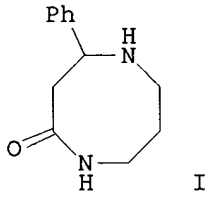
RN 157282-08-1 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-dimethanesulfonic acid, disodium salt, monohydrochloride (9CI) (CA INDEX NAME)



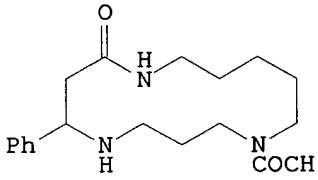
● HCl

●2 Na

L30 ANSWER 56 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:245575 CAPLUS
DOCUMENT NUMBER: 120:245575
TITLE: Study of the transamidative ring expansion of N-ω-halogenoalkyl-β-lactams of alkyl chain lengths 2-12 in liquid ammonia and other liquid amines: syntheses of 7-, 8- and 9-membered 1,5-diaza cyclic ketones, including routes to (±)-dihydroperiphylline and (±)-celabenzine
AUTHOR(S): Begley, Michael J.; Crombie, Leslie; Daigh, David; Jones, Raymond C. F.; Osborne, Steven; Webster, Richard A. B.
CORPORATE SOURCE: Dep. Chem., Univ. Nottingham, Nottingham, NG7 2RD, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1993), (17), 2027-46
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:245575
GI



I



II

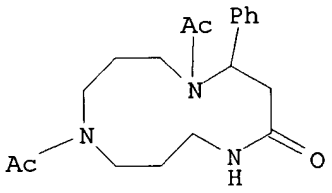
AB N-(3-halogenopropyl)-4-phenylazetidin-2-ones undergo amination in liquid ammonia followed by transamidative ring expansion to give the eight-membered 4-phenyl-1,5-diazacyclooctan-2-one (I) in excellent yield. Ring expansion of the amines in liquid ammonia is found to be much more effective than in hydrocarbon solvents. Formation of 7-, 8-, and 9-membered azalactams from the requisite ω-halogenoalkyl-β-lactams is an excellent synthetic process, though it is not applicable to 10-membered rings. In the cases of rings of 13-, 15- and 17-members, although amination and apparent expansion takes place, the large rings appear not to be stable to ammonia and the final products are acyclic amids. N-[4-halogenobut-2(Z)-enyl]-4-phenylazetidin-2-one satisfactorily forms a 9-membered (Z)-olefinic azalactam, but the (E)-isomer gives an acyclic amino amide. By using alkyl-substituted β-lactam side-chains, C-substituted medium rings can be obtained; the relative instability of N-acyl β-lactams to ammonia, however, leads to acylamino amides rather than expanded rings. Employing ethylamine in place of ammonia, N-ethylated azalactams are formed satisfactorily, and using allylamine, N-allyl medium rings capable of further elaboration are obtained. The chemical of these systems is discussed. Using transamidation in liquid ammonia, a short synthesis of the 9-membered sperimidine alkaloid (±)-dihydroperiphylline (II) was achieved. Synthesis of key intermediates, whose transformation into the 13-membered alkaloids of the celabenzine group has already been effected, has been carried out. X-ray single-crystal structure detns. for 4-phenyl-1,5-diazacyclononan-2-one, trans-4-phenyl-8-methyl-1,5-diazacyclooctan-2-one and (Z)-4-phenyl-1,5-

diazacyclonon-7-en-2-one are reported, and comment is made on certain conformational features.

IT 154218-98-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(intermediate, preparation of diazacyclic ketone)

RN 154218-98-1 CAPLUS

CN 1,5,9-Triazacyclododecan-2-one, 5,9-diacetyl-4-phenyl- (9CI) (CA INDEX NAME)



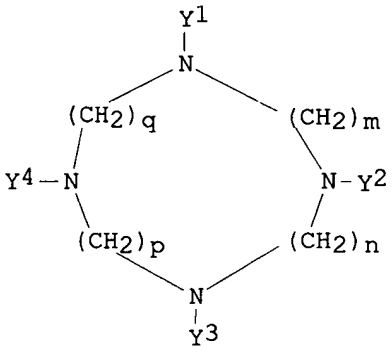
L30 ANSWER 57 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:44581 CAPLUS
DOCUMENT NUMBER: 120:44581
TITLE: Synthesis of polyazamacrocycles with more than one type of side-chain chelating groups
INVENTOR(S): Sherry, A. Dean; Van, Westrenen Jeroen
PATENT ASSIGNEE(S): University of Texas System, USA
SOURCE: PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9312097	A1	19930624	WO 1992-US9247	19921027
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
US 5316757	A	19940531	US 1991-808845	19911213
AU 9229124	A1	19930719	AU 1992-29124	19921027
AU 659244	B2	19950511		
EP 618910	A1	19941012	EP 1992-923096	19921027
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, SE				

PRIORITY APPLN. INFO.:

US 1991-808845	A	19911213
US 1984-662075	A2	19841018
US 1987-7729	A2	19870127
US 1988-291053	A2	19881228
US 1989-357193	B2	19890525
US 1990-615619	A2	19901119
WO 1992-US9247	A	19921027

OTHER SOURCE(S): MARPAT 120:44581
GI



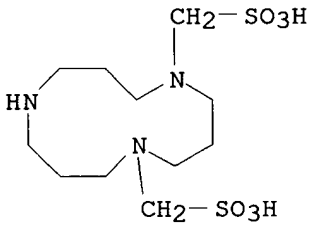
I

AB The pH controlled selectivity of the sulfomethylation reaction is used to prepare a series of di-, tri-, tetra- and hexaazacyclomacrocycles with specified patterns of pendent side-chain chelating groups. The prepared mono and diacetic acid derivs. together with monomethylenephosphonate and

monomethylenephosphinate derivs. of [12]ane N4, [12]aneN3 and [9]aneN3, make these types of ligands easily available by a synthetic pathway that avoids the use of protective groups. A variety of compds., methods and uses are described. Relatively high synthetic yields are reported of polyazamacrocyclic ligands exhibiting a wide and predictable choice of metal ion binding consts. and water and lipid solubilities by reason of their substituent pendent groups. Application is indicated for MRI contrast agents and NMR shift reagents. A method is described for producing a tetraazamacrocycle with selectively N-substituted pendent methylenesulfonate groups having a formula I, where m, n, p and q are independently 2 or 3, and where Y1, Y2, Y3 and Y4 are H or CRyRzSO3-, and at least one of Y1, Y2, Y3 and Y4 is CRyRzSO3-, the method comprising obtaining pKa's for nitrogens of a precursor tetraazamacrocycle where Y1, Y2, Y3 and Y4 are H; reacting, in an aqueous solution having a pH between the lowest pKa of nitrogens to be protonated but not substituted, and the highest pKa of nitrogens to be non-protonated and selectively substituted, the precursor tetraazamacrocycle with a substitution reagent having a formula X-CRYRzSO3- to produce a tetraazamacrocycle with selectively substituted pendent methylenesulfonate groups; wherein X is a leaving group subject to displacement by a non-protonated nitrogen of the precursor tetraazamacrocycle and wherein Ry and Rz are independently hydrogen, alkyl, aryl, alkyl acid, alkyl ether, alkyl ester, or alkyl alc.

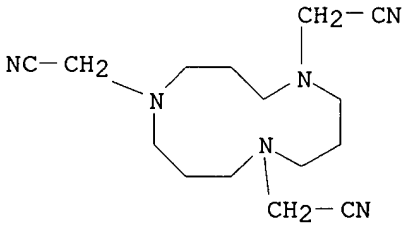
IT 144003-16-7P 144003-25-8P 150263-68-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in polyazamacrocycle preparation for complexes for
magnetic resonance imaging contract agents and NMR shift reagent)

RN 144003-16-7 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-dimethanesulfonic acid, disodium salt (9CI) (CA INDEX NAME)

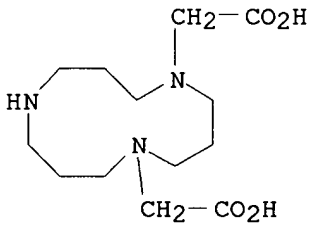


O2 Na

RN 144003-25-8 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triacetonitrile (9CI) (CA INDEX NAME)



RN 150263-68-6 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-diacetic acid, hydrochloride (2:5) (9CI) (CA INDEX NAME)

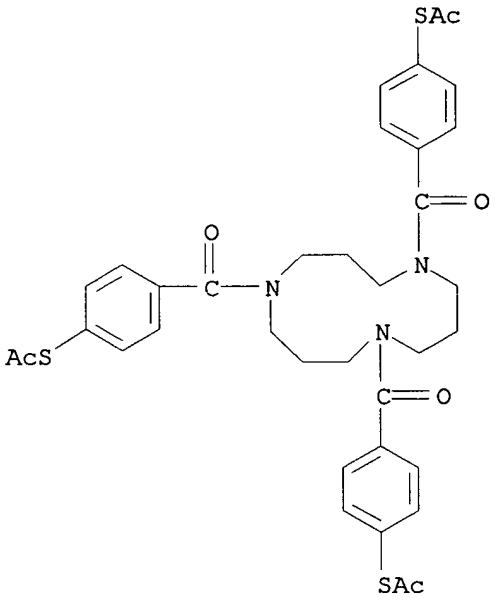


●5/2 HCl

L30 ANSWER 58 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:182041 CAPLUS
DOCUMENT NUMBER: 118:182041
TITLE: Triazacyclane-based trithiols and their use in the preparation of site-differentiated iron-sulfur clusters
AUTHOR(S): Evans, David J.; Garcia, Gabriel; Leigh, G. Jeffery; Newton, Maurice S.; Santana, M. Dolores
CORPORATE SOURCE: Inst. Plant Sci. Res., Univ. Sussex, Brighton, BN1 9RQ, UK
SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1992), (22), 3229-34
CODEN: JCDTBI; ISSN: 0300-9246
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The new tripodal thiol ligands 1,4,7-tris(4-mercaptobenzoyl)-1,4,7-triazacyclononane (H3L) and 1,5,9-tris(4-mercaptobenzoyl)-1,5,9-triazacyclododecane were prepared and characterized. On reaction with Fe-S clusters [Fe4S4(SR)4]2- (R = Et or CMe3), subsite-differentiated clusters, e.g. [Fe4S4L(SEt)]2-, were formed. Site-specific reaction at the differentiated Fe is demonstrated. The novel clusters were prepared both in solution and as isolated solids, and characterized mainly by 1H NMR and Moessbauer spectroscopy.

IT 146070-03-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 146070-03-3 CAPLUS
CN Ethanethioic acid, S,S',S''-[1,5,9-triazacyclododecane-1,5,9-triyltris(carbonyl-4,1-phenylene)] ester (9CI) (CA INDEX NAME)

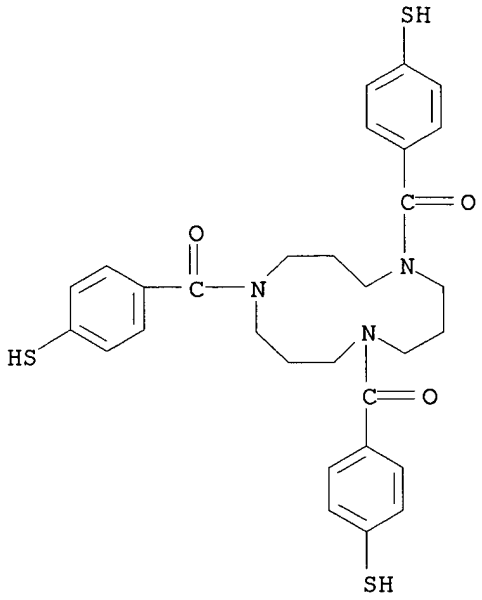


IT 146070-05-5P, 1,5,9-Tris(4-mercaptobenzoyl)-1,5,9-triazacyclododecane
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and substitution reaction of, with iron-sulfur thiolato clusters)

RN 146070-05-5 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris(4-mercaptobenzoyl)- (9CI) (CA INDEX NAME)

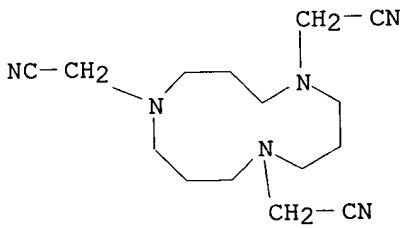


L30 ANSWER 59 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:612468 CAPLUS
DOCUMENT NUMBER: 117:212468
TITLE: Sulfomethylation of di-, tri-, and polyazamacrocycles: a new route to entry of mixed-side-chain macrocyclic chelates
AUTHOR(S): Van Westrenen, Jeroen; Sherry, A. Dean
CORPORATE SOURCE: Dep. Chem., Univ. Texas, Dallas, Richardson, TX, 75083-0688, USA
SOURCE: Bioconjugate Chemistry (1992), 3(6), 524-32
CODEN: BCCHES; ISSN: 1043-1802
DOCUMENT TYPE: Journal
LANGUAGE: English

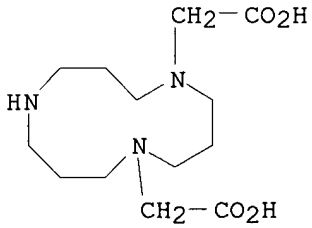
AB The N-sulfomethylation of piperazine and the polyaza macrocycles, [9]aneN3, [12]aneN3, [12]aneN4, and [18]aneN6 with formaldehyde bisulfite in aqueous medium at various pH values is described. The number of methanesulfonate groups introduced into these structures was found to be largely determined by pH. At neutral pH, disubstituted products of [9]aneN3, [12]aneN3, [12]aneN4 are formed and, in the latter case, the trans-1,7-bis(methanesulfonate) isomer was predominant. Similarly, a single, sym. trisubstituted product was formed with [18]aneN6 at neutral pH. Monomethanesulfonated products of these same polyaza compds. were formed at more acidic pH's. These sulfomethylated products were used as an entry into a series of mono- and diacetate, phosphonate, and phosphinate derivs. of [9]aneN3, [12]aneN3, and [12]aneN4. The sulfonate groups may be converted to acetates without isolation of intermediates by using cyanide to displace the sulfonate(s) followed by acidic hydrolysis. The aminomethanesulfonates may also be oxidatively hydrolyzed by using aqueous triiodide as a prelude to the preparation of aminomethanephosphonates or aminomethanephosphinates.

IT 144003-25-8P 144003-27-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 144003-25-8 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triacetonitrile (9CI) (CA INDEX NAME)

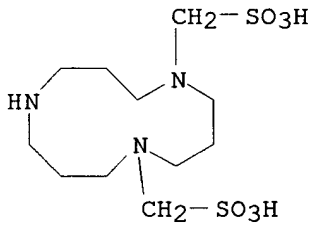


RN 144003-27-0 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-diacetic acid, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT 144003-16-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, substitution with cyanide, and hydroylsis of, aminoacetate from)
RN 144003-16-7 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-dimethanesulfonic acid, disodium salt (9CI) (CA INDEX NAME)



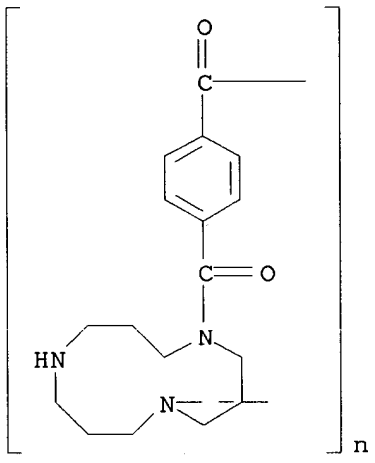
●2 Na

L30 ANSWER 60 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:227097 CAPLUS
DOCUMENT NUMBER: 116:227097
TITLE: Preparation of terephthaloyl and dansyl derivatives of cyclic polyamines and their complexing abilities for metal ions
AUTHOR(S): Fujiwara, Manabu; Matsushita, Takayuki; Wakita, Hisanobu
CORPORATE SOURCE: Fac. Sci. Technol., Ryukoku Univ., Otsu, 520-21, Japan
SOURCE: Analytical Sciences (1991), 7(Suppl., Proc. Int. Congr. Anal. Sci., 1991, Pt. 1), 321-4
CODEN: ANSCEN; ISSN: 0910-6340
DOCUMENT TYPE: Journal
LANGUAGE: English

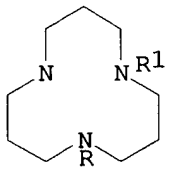
AB Three polymeric ligands containing 9-, 10-, and 12-membered cyclic triamines and four dansyl derivs. of 9-membered cyclic triamine and 12- and 14-membered cyclic tetraamines have been prepared The polymeric ligands can adsorb a copper(II) ion selectively under heterogeneous conditions, and the dansyl derivs. can be applied as a fluorescent reagent to the determination of silver(I) and copper(II) ions.

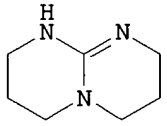
IT 141124-32-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and fluorescence linewidth of, for adsorption and determination of metal ions)

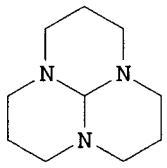
RN 141124-32-5 CAPLUS
CN Poly(1,5,9-triazacyclododecane-1,5-diylcarbonyl-1,4-phenylenecarbonyl) (9CI) (CA INDEX NAME)



L80 ANSWER 61 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:214480 CAPLUS
DOCUMENT NUMBER: 116:214480
TITLE: New synthetic routes to macrocyclic triamines
AUTHOR(S): Alder, Roger W.; Mowlam, Rodney W.; Vachon, David J.; Weisman, Gary R.
CORPORATE SOURCE: Sch. Chem., Univ. Bristol, Bristol, BS8 1TS, UK
SOURCE: Journal of the Chemical Society, Chemical Communications (1992), (6), 507-8
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:214480
GI



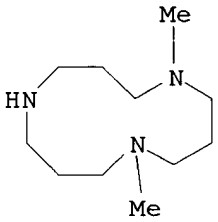
I


II


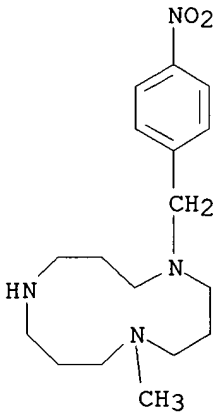
III

AB 1,5,9-Triazacyclododecane I (R = R1 = H) and related macrocyclic triamines can be conveniently constructed around a single carbon atom as template; this route permits the preparation of selectively alkylated derivs. Thus, the reaction of bicyclic guanidine II with 1,3-dibromopropane, followed by reduction of the tricyclic guanidinium salt with LiAlH4 gave orthoamide III. Acid-catalyzed hydrolysis of III gave I (R = R1 = H). Methylation of III with MeI, followed by base-catalyzed hydrolysis gave III (R = Me, R1 = H). Methylation of III with MeI, followed by NaBH4 reduction gave III (R = R1 = Me).

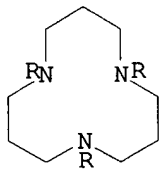
IT 139258-69-8P 141081-92-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 139258-69-8 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-dimethyl- (9CI) (CA INDEX NAME)



RN 141081-92-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1-methyl-5-[(4-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)


NO2
CH2
N
HN
N
CH3

L80 ANSWER 62 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:106266 CAPLUS
DOCUMENT NUMBER: 116:106266
TITLE: Fragmentation during the formic acid/formaldehyde (Eschweiler-Clarke) methylation of polyamines
AUTHOR(S): Alder, Roger W.; Colclough, David; Mowlam, Rodney W.
CORPORATE SOURCE: Sch. Chem., Univ. Bristol, Bristol, BS8 1TS, UK
SOURCE: Tetrahedron Letters (1991), 32(52), 7755-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



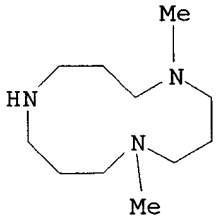
I

AB Eschweiler-Clarke methylations of both acyclic and cyclic polyamines can lead to methylation products of fragments of the original polyamine. Thus, H2N(CH2)3NH(CH2)3NH(CH2)3NH2 yields Me2N(CH2)3NMe2 exclusively and 1,5,9-triazacyclododecane (I, R = H) gives 45% I (R = Me) and 45% Me2N(CH2)3NMe(CH2)3NMe2.

IT 139258-69-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(Eschweiler-Clarke methylation of)

RN 139258-69-8 CAPLUS

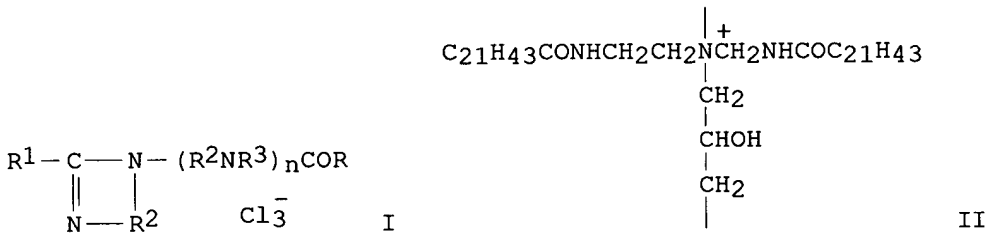
CN 1,5,9-Triazacyclododecane, 1,5-dimethyl- (9CI) (CA INDEX NAME)



L30 ANSWER 63 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:7618 CAPLUS
DOCUMENT NUMBER: 116:7618
TITLE: Synthetic leather sheets having good feel and their manufacture
INVENTOR(S): Tanaka, Noriyuki
PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03193980	A2	19910823	JP 1989-328872	19891218
PRIORITY APPLN. INFO.:			JP 1989-328872	19891218

GI



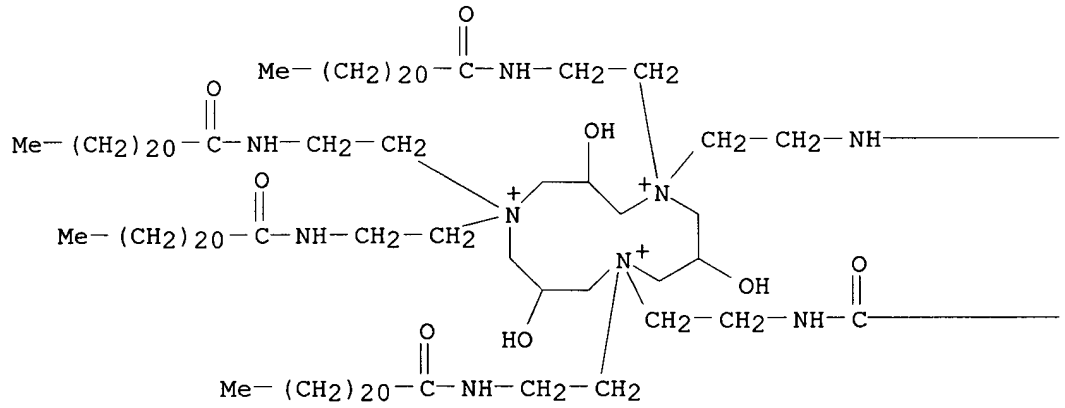
I II

AB Leather-like sheets with good feel and tear strength are prepared by incorporating 0.1-3.0% cationic activating agent to nonwoven sheets (fiber fineness 0.001-3 denier), impregnating with an elastic polymer and wet coagulating, where the activating agent is derived from epichlorohydrin and polyamine derivs. I or R1CONR3(R2NR3)COR (R, R = C11-25 alkyl; R2 = C2-3 alkylene; R3 = H or crosslinking bond; n = 1-8). Needlepunching a mixed web of PET and polyethylene, hot pressing at 120°, removing polyethylene component using C2Cl4, fibrillating, treating with a 0.7% aqueous solution of II, impregnating with 13% DMF solution of polyurethane elastomer, coagulating in a 50/50 aqueous DMF, and puffing gave a 1-mm suede leather substitute.

IT 137955-63-6
RL: USES (Uses)
(activating agents, in manufacture of leather substitutes with good feel and tear strength)

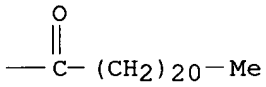
RN 137955-63-6 CAPLUS
CN 1,5,9-Triazoniacyclododecane, 3,7,11-trihydroxy-1,1,5,5,9,9-hexakis[2-[(1-oxodocosyl)amino]ethyl]-, trichloride (9CI) (CA INDEX NAME)

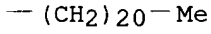
PAGE 1-A



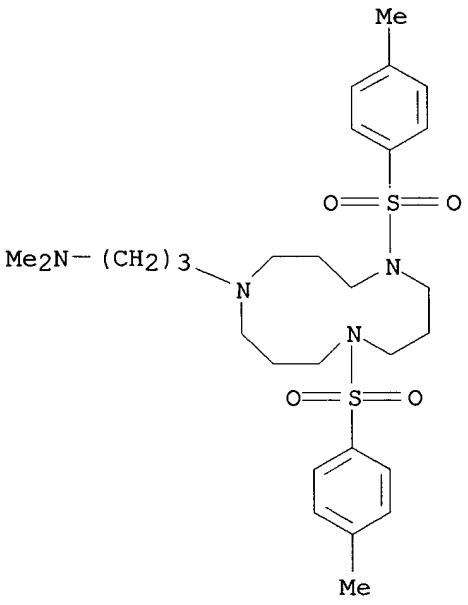
●3 Cl^-

PAGE 1-B

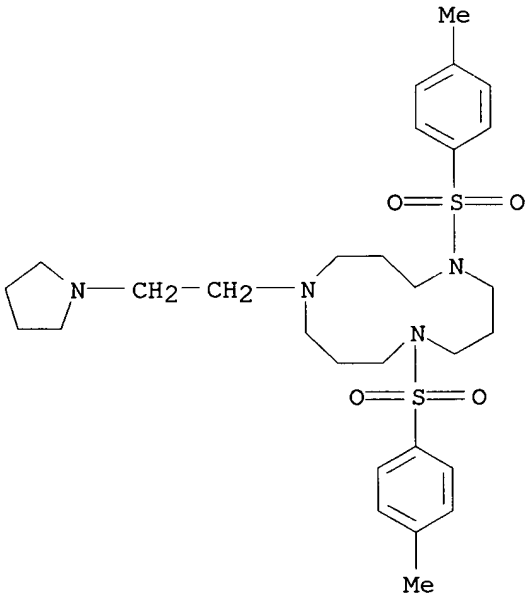




L30 ANSWER 64 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:548941 CAPLUS
DOCUMENT NUMBER: 115:148941
TITLE: Macrocyclic ligands designed to impose tetrahedral coordination: [1-(3-dimethylaminopropyl)-1,5,9-triazacyclododecane], L1, [1{2-(pyrrolidin-1-yl)ethyl}-1,5,9-triazacyclododecane], L2, and their zinc(II) complexes
AUTHOR(S): Alcock, Nathaniel W.; Benniston, Andrew C.; Moore, Peter; Pike, Graham A.; Rawle, Simon C.
CORPORATE SOURCE: Dep. Chem., University of Warwick, Coventry, CV4 7AL, UK
SOURCE: Journal of the Chemical Society, Chemical Communications (1991), (10), 706-8
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
AB L (1-R-1,5,9-triaacyclododecane; R = Me2NCH2CH2CH2, QCH2CH2; Q = pyrrolidin-1-yl) were prepared L reacted with [Zn(DMSO)4](ClO4)2 to yield ZnL(ClO4)2, which were characterized by x-ray crystallog. [Zn(L1)(ClO4)2 (I; L1 = L (R = Me2NCH2CH2CH2)) crystallizes as orthorhombic, space group Pcab, a 15.054(8), b 15.34(1), c 19.25(1) Å, Z = 8, R = 0.0750. [Zn(L2)(OClO3)]ClO4 (II; L2 = L (R = QCH2CH2) crystallizes as orthorhombic, space group Pn21a, a 13.875(13), b 9.811(6), c 16.186(9) Å, Z = 4, R = 0.0570. The Zn in I is approx. tetrahedrally coordinated by L1. The Zn in II has distorted trigonal bipyramid coordination by L2 and OClO3-.
IT 135787-24-5P 135787-25-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and detosylation of)
RN 135787-24-5 CAPLUS
CN 1,5,9-Triazacyclododecane-1-propanamine, N,N-dimethyl-5,9-bis[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 135787-25-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5-bis[(4-methylphenyl)sulfonyl]-9-[2-(1-pyrrolidinyl)ethyl]- (9CI) (CA INDEX NAME)



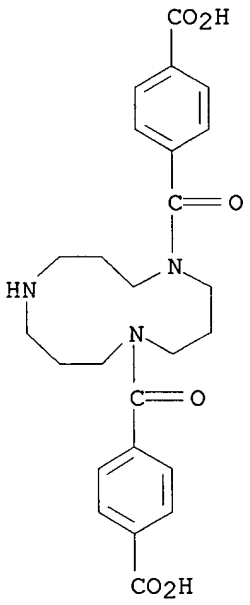
L30 ANSWER 65 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:109632 CAPLUS
DOCUMENT NUMBER: 114:109632
TITLE: Preparation of terephthaloyl derivatives of cyclic triamines and their selectivities toward copper(II), nickel(II) and zinc(II) ions
AUTHOR(S): Fujiwara, Manabu; Matsuda, Jun; Wakita, Hisanobu
CORPORATE SOURCE: Fac. Sci., Fukuoka Univ., Fukuoka, 814-01, Japan
SOURCE: Polyhedron (1990), 9(20), 2491-5
CODEN: PLYHDE; ISSN: 0277-5387
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Three polymeric ligands containing 9-, 10- and 12-membered cyclic triamines were prepared by the reaction of cyclic triamine with terephthaloyl chloride. They are insol. in water and ordinary organic solvents, but under heterogeneous conditions they can adsorb some transition metal ions [Cu(II), Ni(II), and Zn(II)] very rapidly. The complexing abilities of the 9- and 10-membered polymeric ligands are stronger in the order Zn < Ni < Cu, but that of the 12-membered polymeric ligand is Ni < Zn < Cu.

IT 132434-02-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and selective capacity for transition metals of)
RN 132434-02-7 CAPLUS
CN Benzoic acid, 4,4'-(1,5,9-triazacyclododecane-1,5-diyldicarbonyl)bis-, homopolymer (9CI) (CA INDEX NAME)

CM 1

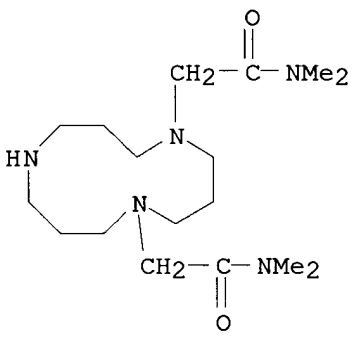
CRN 132434-01-6
CMF C25 H29 N3 O6



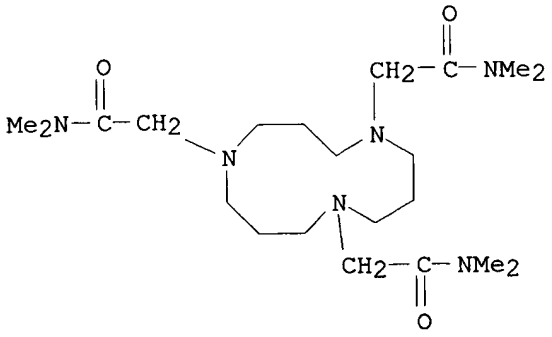
L30 ANSWER 66 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:30923 CAPLUS
DOCUMENT NUMBER: 114:30923
TITLE: Synthesis and binding properties of amide-functionalized polyaza macrocycles
AUTHOR(S): Kataky, Ritu; Matthes, Karen E.; Nicholson, Patrick E.; Parker, David; Buschmann, Hans J.
CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, DH1 3LE, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1990), (8), 1425-32
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:30923

AB A series of amide N-functionalized coronands was prepared based on parent [9]-N3, [12]-N3, [12]-N2O2, and [12]-N4 polyazamacrocycles. Complexation with alkali and alkaline earth cations, particularly Li+, Na+, and Ca2+, was monitored by using 13C NMR and IR spectroscopy, fast-atom-bombardment mass spectrometry, calorimetric, and potentiometric anal. in aqueous and alc. media. Particularly strong complexation in H2O was observed for Ca2+ with 1,4,7,10-tetrakis(N,N-dimethylacetamido)-1,4,7,10-tetraazacyclododecane (log Ks = 6.82 [H2O, 298 K]), and selective Ca2+ complexation was observed with 1,7-dioxa-4,10-bis(dimethylethanamido)-4,10-diazacyclododecane.

IT 127603-39-8
RL: PRP (Properties)
(acid dissociation consts. of)
RN 127603-39-8 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-diacetamide, N,N,N',N'-tetramethyl- (9CI) (CA INDEX NAME)



IT 127603-41-2D, lithium and sodium complexes
RL: PRP (Properties)
(selectivity in formation and stability consts. of)
RN 127603-41-2 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triacetamide, N,N,N',N',N'',N''-hexamethyl- (9CI) (CA INDEX NAME)

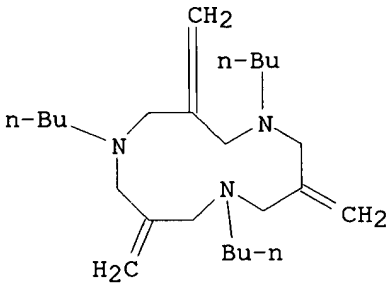


L30 ANSWER 67 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:7349 CAPLUS
DOCUMENT NUMBER: 114:7349
TITLE: Polycondensation catalyzed by palladium complex. III. Syntheses of linear polyamines and cyclic oligoamines via π-allyl palladium intermediates
AUTHOR(S): Suzuki, Masato; Lim, Jong Chan; Oguni, Masahiro; Eberhardt, Anke; Saegusa, Takeo
CORPORATE SOURCE: Fac. Eng., Kyoto Univ., Kyoto, 606, Japan
SOURCE: Polymer Journal (Tokyo, Japan) (1990), 22(9), 815-25
CODEN: POLJB8; ISSN: 0032-3896
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Polyamines were prepared by polymerization of bifunctional allylic compds. with diamines or monoamines in the presence of Pd complexes. Tosylated amines were also used to produce the corresponding tosylated derivs. of polyamines. The monomer structure and the character of the catalyst influenced the proportion between linear and cyclic products.

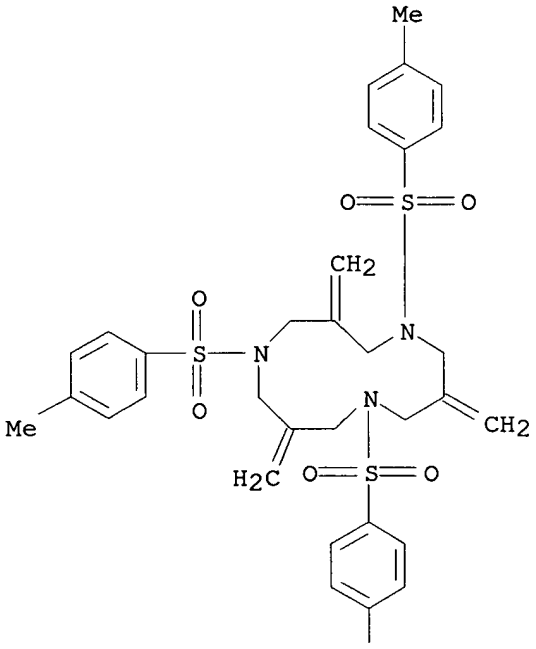
IT 130927-29-6P 130927-35-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 130927-29-6 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tributyl-3,7,11-tris(methylene)- (9CI) (CA INDEX NAME)



RN 130927-35-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 3,7,11-tris(methylene)-1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

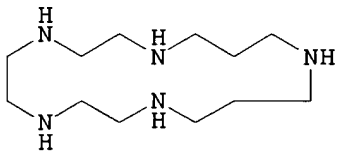
PAGE 1-A



PAGE 2-A

L30 ANSWER 68 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:571994 CAPLUS
DOCUMENT NUMBER: 113:171994
TITLE: Macroheterocycles. 51. Synthesis of macrocyclic polyamines in a two-phase system
AUTHOR(S): Luk'yanenko, N. G.; Basok, S. S.; Filonova, L. K.; Kulikov, N. V.; Pastushok, V. N.
CORPORATE SOURCE: Fiz.-Khim. Inst., Odessa, 270080, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1990), (3), 401-4
CODEN: KGSSAQ; ISSN: 0453-8234
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 113:171994
GI



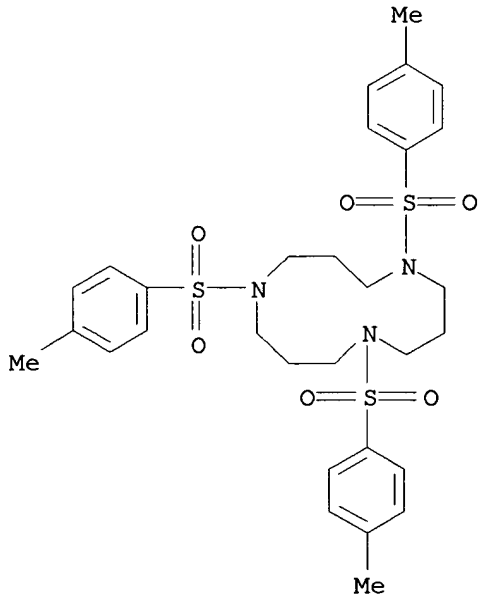
I

AB A new convenient synthesis of macrocyclic polyamines e.g., (I) based on condensation of bis(sulfonamides) with bis(tosylates) or dibromides in a two-phase toluene(xylene)-aqueous NaOH system gives the title compds. in 65-90% yield.

IT 35980-67-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and detosylation of)

RN 35980-67-7 CAPLUS

CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)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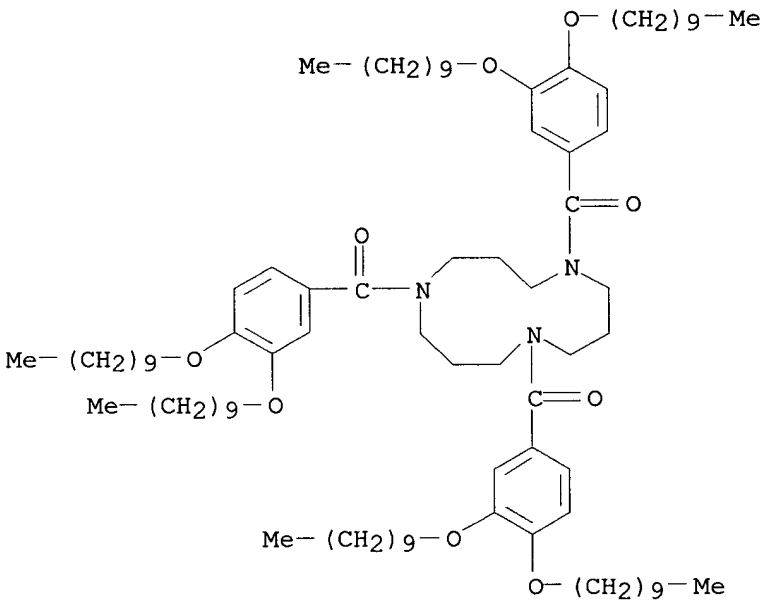
Me

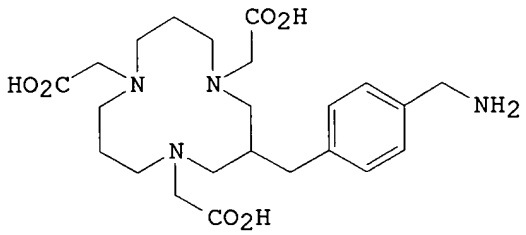
L30 ANSWER 69 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:563133 CAPLUS
DOCUMENT NUMBER: 113:163133
TITLE: Liquid crystalline azamacrocyclic derivatives
AUTHOR(S): Lattermann, G.
CORPORATE SOURCE: Univ. Bayreuth, Bayreuth, D-8580, Germany
SOURCE: Molecular Crystals and Liquid Crystals (1990), 182B, 299-311
CODEN: MCLCA5; ISSN: 0026-8941
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Three examples of new liquid crystalline compds. with azamacrocyclic cores are described. Apart from a substituted hexacyclene with 12 alkoxy sidechains, 2 triazacrown ether derivs. are presented. Their discotic mol. shape causes mesomorphic behavior, which is characterized by DSC-measurements and polarizing microscopy. Water absorption from air can slightly modify the transition temps. The triazamacocyclic derivs. exhibit a strongly hindered recrystn.; their glass transition temps. are above room temperature

IT 129820-26-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(liquid crystal, preparation and transition temps. of)
RN 129820-26-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris[3,4-bis(decyloxy)benzoyl]- (9CI) (CA INDEX NAME)



L80 ANSWER 70 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:423877 CAPLUS
DOCUMENT NUMBER: 113:23877
TITLE: Syntheses of C- and N-functionalized derivatives of 1,5,9-triazacyclododecane
AUTHOR(S): Helps, Ian M.; Parker, David; Jankowski, Karl J.; Chapman, James; Nicholson, Patrick E.
CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, DH1 3LE, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1989), (11), 2079-82
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:23877
GI



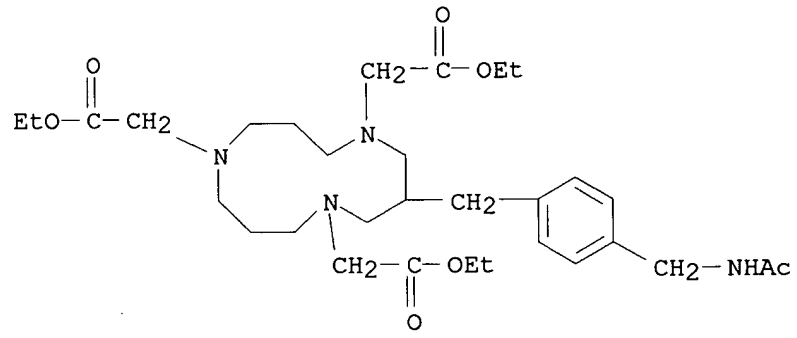
I

AB The synthesis of a series of di- and tri-N-substituted triazacyclododecane ligands has been effected through the intermediacy of monotosylamide derivs. A C-functionalized aminobenzyl [12]-N3 tris(carboxymethyl) derivative I has been prepared permitting subsequent linkage to a protein.

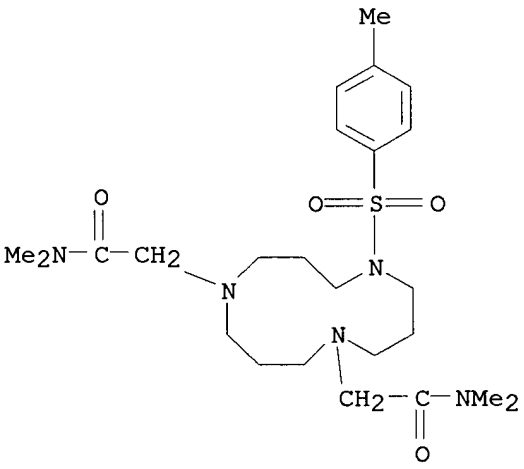
IT 124659-34-3P 127603-38-7P 127603-40-1P
127647-89-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 124659-34-3 CAPLUS

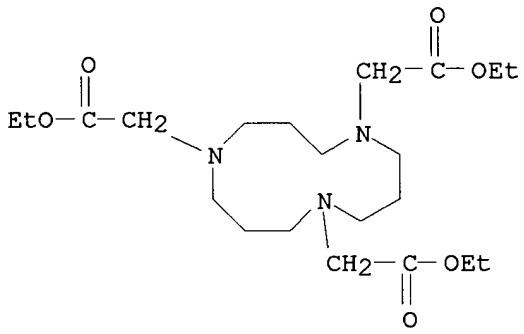
CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-[(acetylamino)methyl]phenyl]methyl]-, triethyl ester (9CI) (CA INDEX NAME)



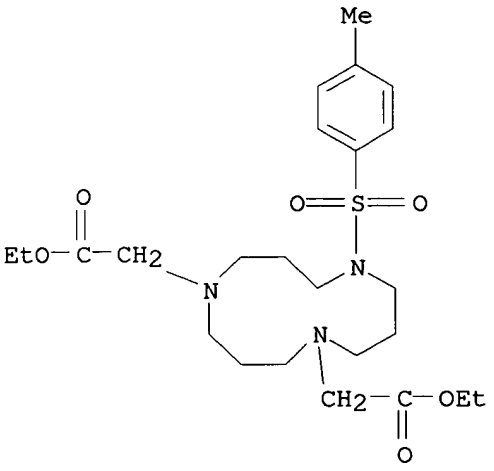
RN 127603-38-7 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-diacetamide, N,N,N',N'-tetramethyl-9-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



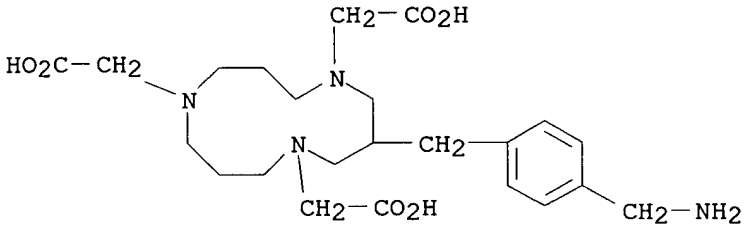
RN 127603-40-1 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, triethyl ester (9CI) (CA INDEX NAME)



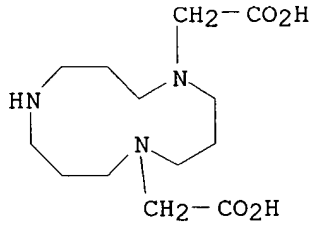
RN 127647-89-6 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-diacetic acid, 9-[(4-methylphenyl)sulfonyl]-, diethyl ester (9CI) (CA INDEX NAME)



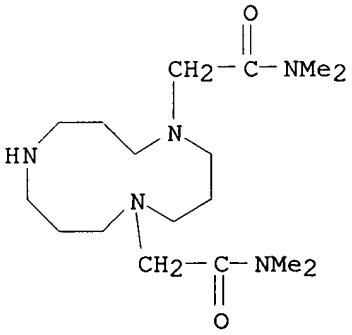
IT 124659-35-4P 127603-37-6P 127603-39-8P
127603-41-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 124659-35-4 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-(aminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



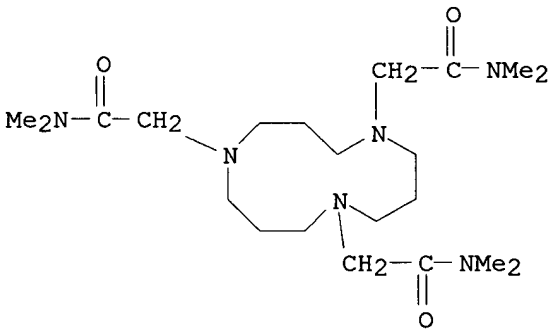
RN 127603-37-6 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-diacetic acid (9CI) (CA INDEX NAME)



RN 127603-39-8 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5-diacetamide, N,N,N',N'-tetramethyl- (9CI) (CA INDEX NAME)



RN 127603-41-2 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triacetamide, N,N,N',N',N'',N''-hexamethyl- (9CI) (CA INDEX NAME)



L30 ANSWER 71 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:118864 CAPLUS
DOCUMENT NUMBER: 112:118864
TITLE: Tri-aza macrocycles and metal complexes thereof, their preparation and use in diagnostic imaging and therapy
INVENTOR(S): Parker, David; Millican, Thomas Andrew
PATENT ASSIGNEE(S): Celltech Ltd., UK
SOURCE: PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8901475	A1	19890223	WO 1988-GB672	19880812
W: AU, DK, JP, KR, US				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AU 8822527	A1	19890309	AU 1988-22527	19880812
AU 629178	B2	19921001		
EP 329737	A1	19890830	EP 1988-906973	19880812
EP 329737	B1	19950412		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 02501069	T2	19900412	JP 1988-506687	19880812
AT 121082	E	19950415	AT 1988-906973	19880812
CA 1340603	A1	19990622	CA 1988-574629	19880812
DK 8901728	A	19890411	DK 1989-1728	19890411
US 5247075	A	19930921	US 1991-784601	19911022
US 5484893	A	19960116	US 1993-78650	19930621
PRIORITY APPLN. INFO.:			GB 1987-19041 A	19870812
			WO 1988-GB672 A	19880812
			US 1989-363683 B1	19890609
			US 1991-784601 A3	19911022

OTHER SOURCE(S): MARPAT 112:118864
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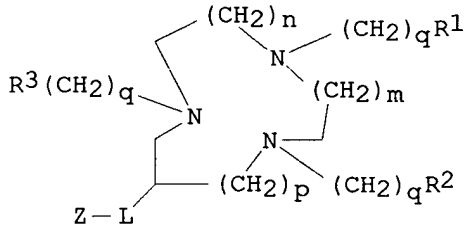
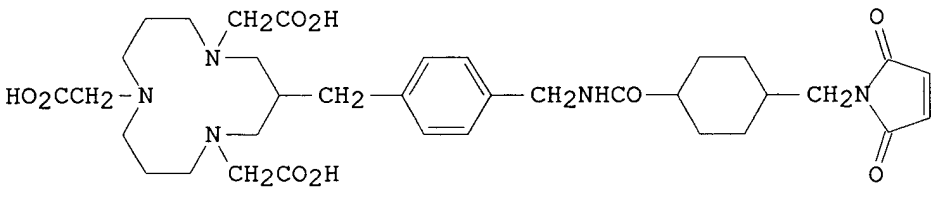


I



II

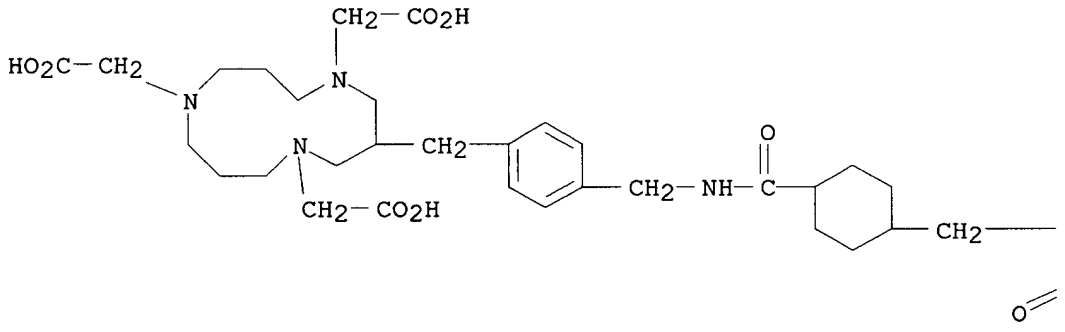
AB Triazacycloalkane derivs. I (m, n = 0-3; p = 0-2; q = 0-6; R1-R3 = H, alkyl, alkoxyalkyl, CO2H, SO3H, PO3H2, aryl; L = bond, linker; Z = H, reactive functional group) and their metal complexes and salts are prepared for use in diagnostic imaging and treatment of abnormal cell disorders, e.g. tumors. I are particularly suitable for coupling to other mols. such as proteins for these applications. Thus, II was prepared in 8 steps from p-cyanobenzyldiethyl malonate and 1,7-diamino-4-azaheptane, converted to the 111In complex, and conjugated with monoclonal antibody B72.3. When injected into mice, this conjugate showed high persistence in the tissues (≈65% of injected dose after 24 h), mainly in the blood (47.52%).

IT 124659-23-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conjugation with monoclonal antibody for neoplasm inhibition and scintigraphy)

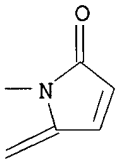
RN 124659-23-0 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-[[[[4-[(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)methyl]cyclohexyl]carbonyl]amino]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

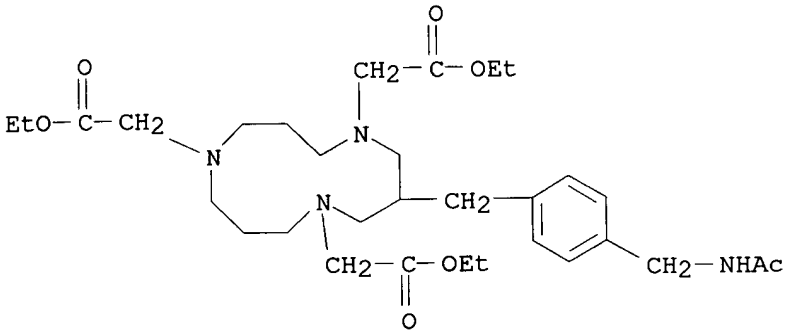


IT 124659-34-3P 124659-35-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, in triazacyclononane derivative metal complex preparation as imaging
agent and neoplasm inhibitor)

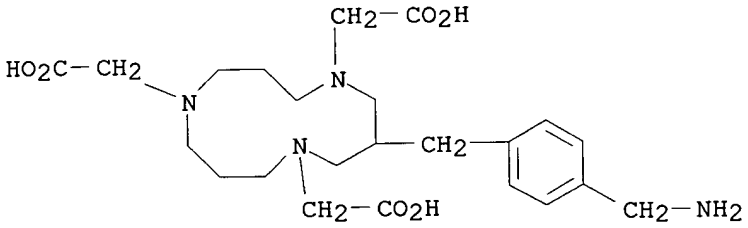
RN 124659-34-3 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-

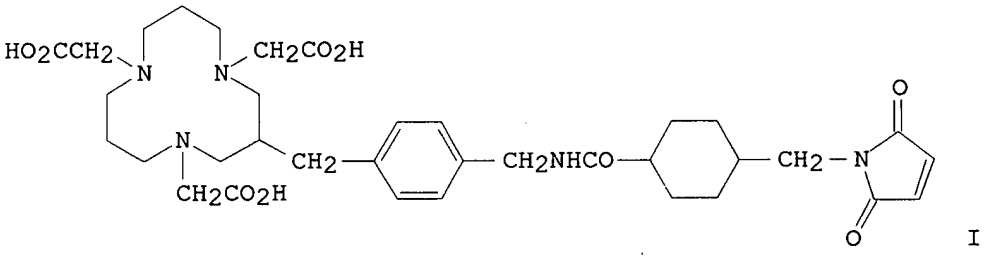
[(acetylamino)methyl]phenyl]methyl]-, triethyl ester (9CI) (CA INDEX NAME)



RN 124659-35-4 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-(aminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



L30 ANSWER 72 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:55813 CAPLUS
DOCUMENT NUMBER: 112:55813
TITLE: Towards tumor imaging with indium-111 labeled macrocycle-antibody conjugates
AUTHOR(S): Craig, Andrew S.; Helps, Ian M.; Jankowski, Karl J.; Parker, David; Beeley, Nigel R. A.; Boyce, Byron A.; Eaton, Michael A. W.; Millican, Andrew T.; Millar, Kenneth; et al.
CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, DH1 3LE, UK
SOURCE: Journal of the Chemical Society, Chemical Communications (1989), (12), 794-6
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:55813
GI



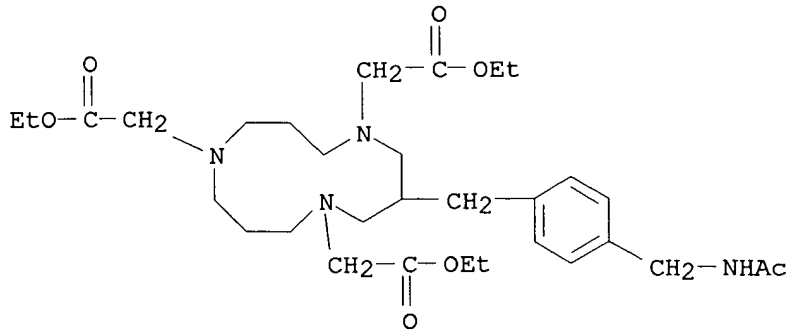
I

AB C-Functionalized triazacyclododecane and triazacyclononane triacid macrocycles, e.g. I, have been prepared and covalently attached to a monoclonal antibody and may be labeled with 111In to form kinetically inert radiolabeled complexes.

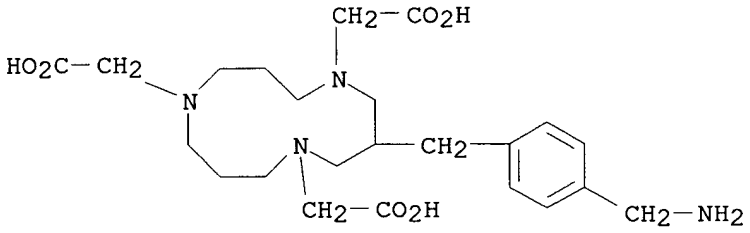
IT 124659-34-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acid hydrolysis of)

RN 124659-34-3 CAPLUS

CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-[(acetylamino)methyl]phenyl]methyl]-, triethyl ester (9CI) (CA INDEX NAME)

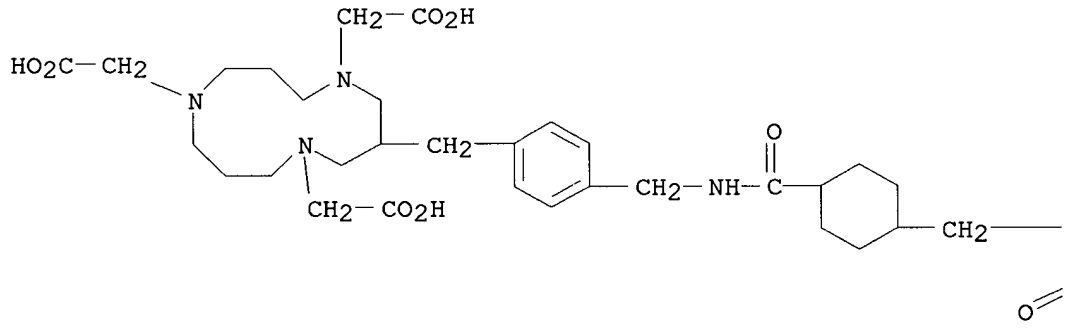


IT 124659-35-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amidation by, of (carboxycyclohexylmethyl)maleimide)
RN 124659-35-4 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-(aminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

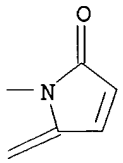


IT 124659-23-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation of, with indium-111 trichloride)
RN 124659-23-0 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, 3-[[4-[[[[4-[(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)methyl]cyclohexyl]carbonyl]amino]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

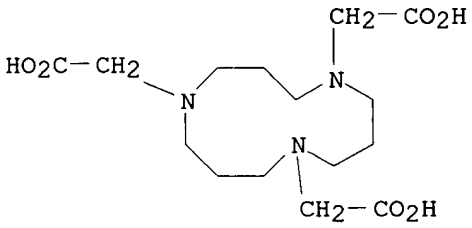


L80 ANSWER 73 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:26399 CAPLUS
DOCUMENT NUMBER: 112:26399
TITLE: Potentiometry and NMR studies of 1,5,9-triazacyclododecane-N,N',N''-triacetic acid and its metal ion complexes
AUTHOR(S): Cortes, S.; Brucher, E.; Geraldes, C. F. G. C.; Sherry, A. D.
CORPORATE SOURCE: Univ. Texas, Dallas, Richardson, TX, 75083-0688, USA
SOURCE: Inorganic Chemistry (1990), 29(1), 5-9
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new chelating macrocycle, 1,5,9-triazacyclododecane-N,N',N''-triacetic acid (DOTRA), has been synthesized, and its complexes with Zn2+, Cd2+, Ca2+, Mg2+, and Mn2+ have been examined by potentiometry and NMR spectroscopy. The first protonation constant of the free ligand (log K1 = 12.8) was determined spectrophotometrically, while the remaining were evaluated from potentiometric data (log K2 = 7.55, log K3 = 3.65, log K4 = 2.1). DOTRA forms complexes with Mn2+, Mg2+, and Ca2+ rather slowly but reacts much more rapidly with Zn2+ and Cd2+. As reported previously for the nine-membered-ring triaza analog NOTA, DOTRA also forms a more stable complex with Mg2+ than with Ca2+ (log Kst = 7.1 vs. 6.0). High-resolution NMR spectra of the Zn2+, Cd2+, and Mg2+ complexes (log Kst = 19.0, 15.7, and 7.1, resp.) indicate the three six-membered chelate rings are sym. and quite rigid in aqueous solution, as evidenced by nonequivalence of all six chelate ring protons.

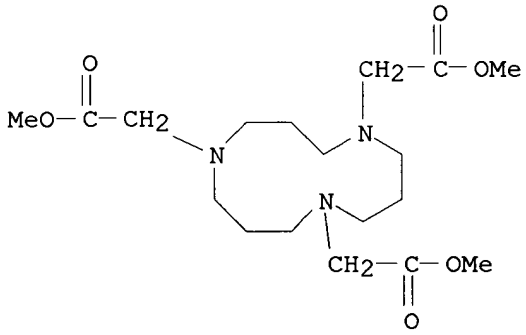
IT 123726-20-5P 123726-21-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 123726-20-5 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, trihydrochloride (9CI) (CA INDEX NAME)



⊛3 HCl

RN 123726-21-6 CAPLUS
CN 1,5,9-Triazacyclododecane-1,5,9-triacetic acid, trimethyl ester (9CI) (CA INDEX NAME)



L80 ANSWER 74 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:407379 CAPLUS
DOCUMENT NUMBER: 111:7379
TITLE: A simplified synthetic route to polyaza macrocycles
AUTHOR(S): Chavez, F.; Sherry, A. D.
CORPORATE SOURCE: Dep. Chem., Univ. Texas, Dallas, Richardson, TX, 75083-0688, USA
SOURCE: Journal of Organic Chemistry (1989), 54(12), 2990-2
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:7379
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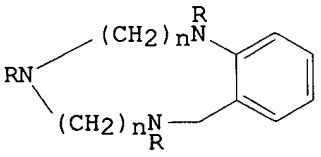

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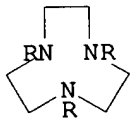
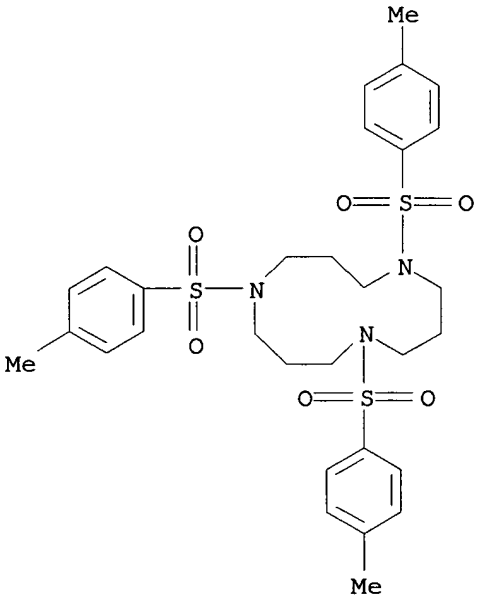


II

AB A simple, low-cost procedure for the preparation of small to medium-sized polyazamacrocycles, e.g. I (n = 2, 3,; R = tosyl) and II (R = tosyl) is reported. It involves base deprotonation of a linear polyazatosylamide by finely ground K2CO3 in dry DMF followed by slow addition of a dibromoalkane at or near room temperature The reaction may be run at final concns. approaching 0.1M on gram or multigram scales and with yields, after isolation and recrystn., approaching 90%.

IT 35980-67-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35980-67-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)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L20 ANSWER 75 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:407370 CAPLUS
DOCUMENT NUMBER: 111:7370
TITLE: Macroheterocycles. Part 44. Facile synthesis of azacrown ethers and cryptands in a two-phase system
AUTHOR(S): Lukyanenko, N. G.; Basok, S. S.; Filonova, L. K.
CORPORATE SOURCE: A. V. Bogatskii Phys.-Chem. Inst., Odessa, 270080, USSR
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1988), (12), 3141-7
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:7370
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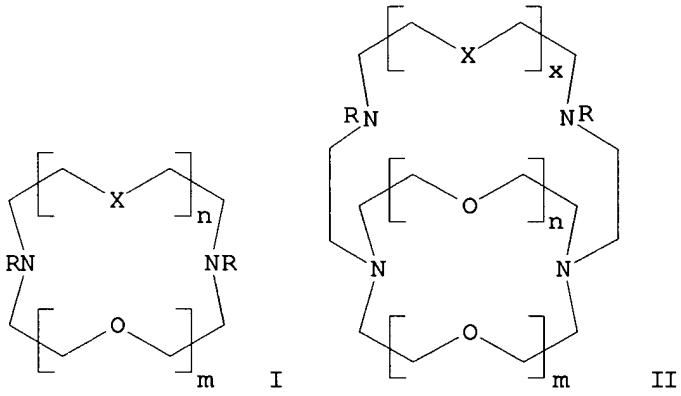
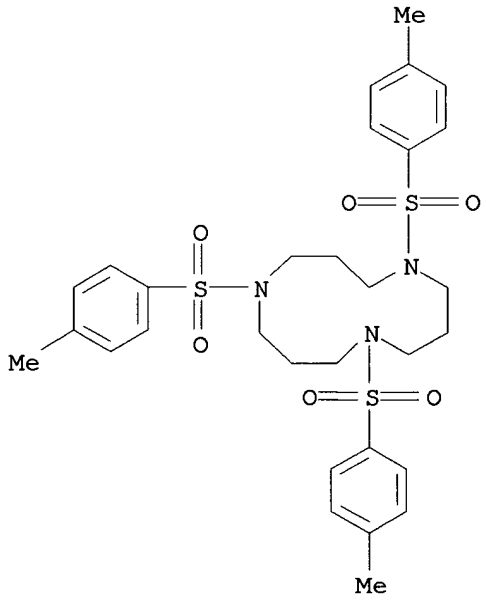


AB A facile procedure is proposed for the preparation of azacrown ethers, e.g., I (X = O, NR; R = tosyl, n, m = 1,2,3) and cryptands, e.g., II (X = O, NR; R = tosyl, n, m, x = 1,2) by condensation of dibromides or ethylene glycol bis(toluene-p-sulfonate) with acyclic bis(sulfonamide)s or with bis[2-(p-tolylsulfonylamino)ethyl]diazacrown ethers, resp. The reaction was carried out in a two-phase system of aqueous alkali-toluene (benzene) in the presence of quaternary ammonium salts as phase transfer catalysts. The catalytic activity decreased in the sequence: Bu4Nl ≈ Bu4NBr > Bu4NCl > Bu4NHSO4 > Et3CH2C6H5NCl. Maximum yields of twelve-membered azacrown ethers are obtained when lithium hydroxide is used, while crown ethers of larger size are observed in the presence of sodium or potassium hydroxides; this may be due to a template effect.

IT 35980-67-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and detosylation of)

RN 35980-67-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)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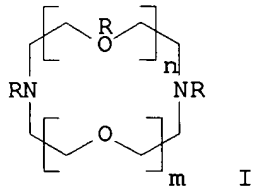
L30 ANSWER 76 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:231598 CAPLUS
DOCUMENT NUMBER: 110:231598
TITLE: Macroheterocycles. XXXVI. Convenient synthesis of di- and polyaza crown ethers
AUTHOR(S): Luk'yanenko, N. G.; Bosok, S. S.; Filonova, L. K.
CORPORATE SOURCE: Fiz.-Khim. Inst. im. Bogatskogo, Odessa, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1988), 24(8), 1731-42
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 110:231598
GI

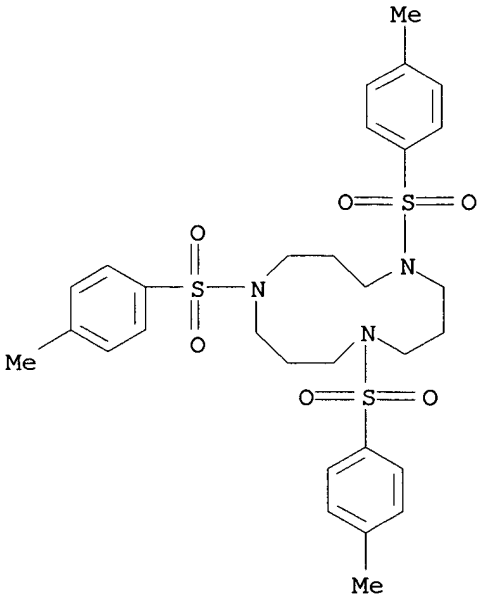


I

AB Di- and polyaza crown ethers, e.g. I (R = tosyl, H, n, m = 0-8) were prepared by condensation of bissulfonamides with dibromides and ditosylates in a 2-phase system containing aqueous base and either toluene or C6H6. The optimum concentration range for the substrate and alkylating agent are 0.017-0.1 mol/L. The catalytic activity of the quaternary ammonium salts decrease in the series: Bu4NI ≥ Bu4NCl > Bu4NHSO4 > Et3PhCH2NCl ≥ Et4NI > Et4NBr. The maximum yield of 12 crown ethers were obtained with LiOH solns.; with the remainder NaOH and KOH are favored.

IT 35980-67-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 35980-67-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)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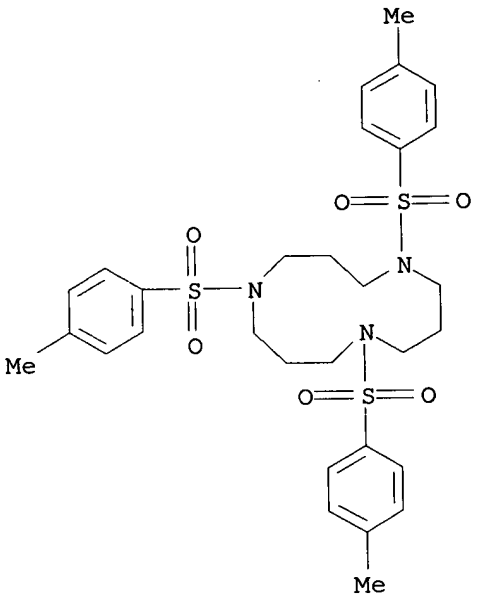
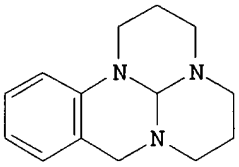
L80 ANSWER 77 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:94528 CAPLUS
DOCUMENT NUMBER: 108:94528
TITLE: Synthesis and copper(I) complexes of a series of 9- to 13-membered N3 macrocycles
AUTHOR(S): Briellmann, Markus; Kaderli, Susan; Meyer, Charles J.; Zuberbuhler, Andreas D.
CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Basel, Basel, CH-4056, Switz.
SOURCE: Helvetica Chimica Acta (1987), 70(3), 680-9
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:94528
GI For diagram(s), see printed CA Issue.
AB Eight cyclic triamines with ring sizes between 9 and 13 (I, n = 2, m = 2-6; n = 3, m = 2-4) were prepared by cyclocondensation of the appropriate triamine tritosylate with the appropriate ditosylate and subsequent detosylation of the macrocyclic triamine tritosylates.
IT 35980-67-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and detosylation of, with sulfuric acid)
RN 35980-67-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



L30 ANSWER 78 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:75328 CAPLUS
DOCUMENT NUMBER: 108:75328
TITLE: Synthesis of 2,3,5,6-tetrahydro-1H,4H,11cH-3a,6a,11b-triazabenz[de]anthracene (I) and x-ray crystal structure determinations of I, hexahydro-1H,4H,7H,9bH-3a,6a,9a-triazaphenalene, N,N',N"-tritosylbenzo[b]-[1,5,9]-triazacyclododecane, and of N,N',N"-tritosyl-1,5,9-triazacyclododecane
AUTHOR(S): Beddoes, Roy L.; Edwards, W. D.; Joule, J. A.; Mills, O. S.; Street, J. D.
CORPORATE SOURCE: Chem. Dep., Manchester Univ., Manchester, M13 9PL, UK
SOURCE: Tetrahedron (1987), 43(8), 1903-20
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:75328
GI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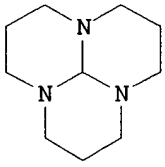
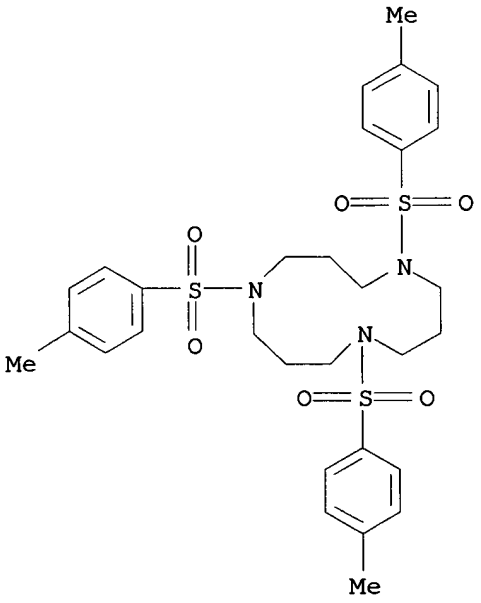

II

AB Triazabenz[de]anthracene I was prepared from anthranilonitrile. X-ray crystal structure detns. on triazaphenalene II and its benzo analog I show them to adopt differing conformations; the reasons for this are discussed.
IT 35980-67-7
RL: PRP (Properties)
(crystal structure of)
RN 35980-67-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)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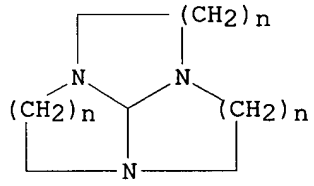
L30 ANSWER 79 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:56096 CAPLUS
DOCUMENT NUMBER: 108:56096
TITLE: Selective N-protection of medium-ring triamines
AUTHOR(S): Weisman, Gary R.; Vachon, David J.; Johnson, Van B.; Gronbeck, Dana A.
CORPORATE SOURCE: Dep. Chem., Univ. New Hampshire, Durham, NH, 03824, USA
SOURCE: Journal of the Chemical Society, Chemical Communications (1987), (12), 886-7
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:56096
GI



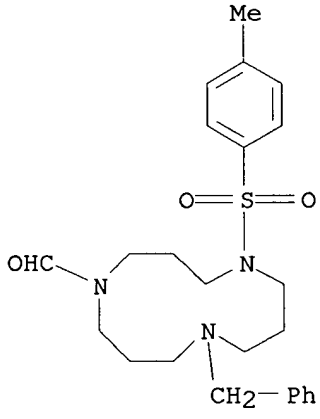
I

AB Efficient methods for selective N-protection of 1,4,7-triazacyclononane and 1,5,9-triazacyclododecane and for the synthesis of related bis(coronands) based upon the synthetic intermediacy of tricyclic ortho amides I (n = 1, 2) were developed.

IT 112498-56-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of, by sodium hydroxide)

RN 112498-56-3 CAPLUS

CN 1,5,9-Triazacyclododecane-1-carboxaldehyde, 5-[(4-methylphenyl)sulfonyl]-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

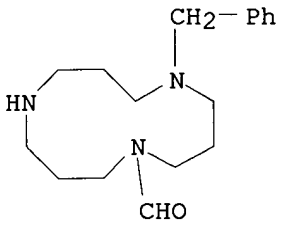


IT 112498-55-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and N-tosylation of)

RN 112498-55-2 CAPLUS

CN 1,5,9-Triazacyclododecane-1-carboxaldehyde, 5-(phenylmethyl)- (9CI) (CA INDEX NAME)

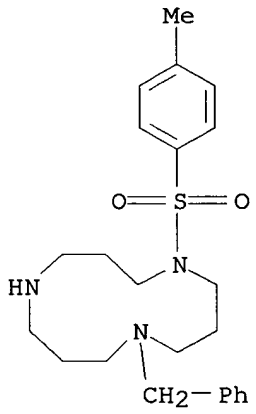


IT 112498-57-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 112498-57-4 CAPLUS

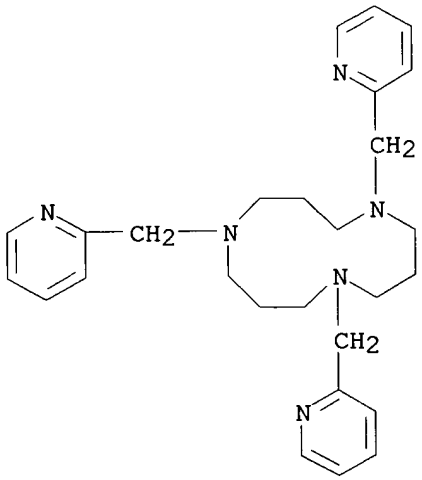
CN 1,5,9-Triazacyclododecane, 1-[(4-methylphenyl)sulfonyl]-5-(phenylmethyl)- (9CI) (CA INDEX NAME)



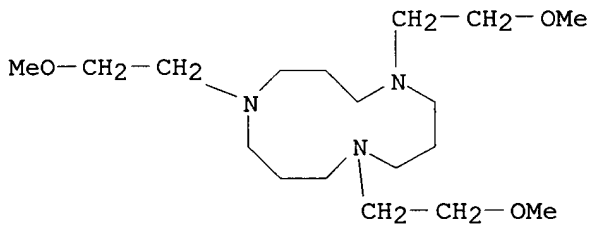
L30 ANSWER 80 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:471514 CAPLUS
DOCUMENT NUMBER: 105:71514
TITLE: Synthesis and structure of metal complexes of triaza macrocycles with three pendant pyridylmethyl arms
AUTHOR(S): Christiansen, Lise; Hendrickson, David N.; Toftlund, Hans; Wilson, Scott R.; Xie, Chuan Liang
CORPORATE SOURCE: Dep. Chem., Univ. Odense, Odense, DK-5230, Den.
SOURCE: Inorganic Chemistry (1986), 25(16), 2813-18
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

AB [ML](ClO4)2 and [CoL](ClO4)3 (L = 2,5,8-tris(2-pyridylmethyl)-2,5,8-triazanonane (L1); 1,4,7-tris(2-pyridylmethyl)-1,4,7-triazacyclononane (L2), 1,5,9-tris(2-pyridylmethyl)-1,5,9-triazacyclododecane (L3)) and the ligands were prepared The x-ray structure of [FeL2](ClO4)2 was determined by using Patterson methods, in conjunction with data measured on a 4-circle diffractometer, to give discrepancy factors of RF = 0.041 and RwF = 0.052 for 1841 observed (I > 2.58σ(I)) reflections. The compound crystallizes in the trigonal space group P3 with Z = 3, a 16.978(3) and c 7.909(3) Å. There are 3 crystallog. independent FeL2 cations; each cation has a C3 axis perpendicular to the plane of the 3 pyridine N atoms as well as the plane of the 3 aliphatic N atoms of a L2 ligand. All 3 cations have similar dimensions; the bond distances are appropriate for a low-spin Fe(II) complex, a description that is in agreement with the variable-temperature Moessbauer and magnetic susceptibility data that were obtained. The ClO4- and SbF6- salts of [FeL1]2+ and [FeL3]2+ are high-spin Fe(II) compds. Electronic absorption spectral data are presented for the [ML](ClO4)2 and [CoL](ClO4)3 in solution to show that the [FeL2]2+ complex is close to the spin-crossover point. The interrelations between the kinetics of reactions such as racemization and the possibility of converting from low spin to high spin, i.e. the existence of the spin-crossover phenomenon, are examined for the L2 complex. 13C NMR results are presented to show that [FeL2]2+ undergoes a relatively rapid racemization with a rate constant in excess of 150 s-1 at 90°. The P3 is a polar space group, so the Fe(II) cations in [FeL2](ClO4)2 are 1 of an enantiomeric pair; i.e., the cations are optically active and resolved. The kinetics of racemization that develop after a crushed large single crystal is dissolved, monitored with a CD spectrometer, give a rate constant of k = 2.7 + 10-3 s-1 at 5°. The racemization takes place via an intramol. twist mechanism and such a mechanism is strongly favored by having a situation where the triplet excited state is close in energy to the singlet ground state of an Fe(II) complex.

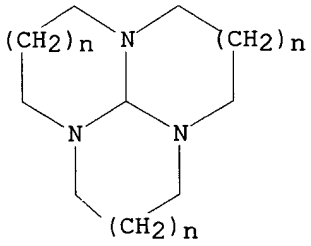
IT 102851-51-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 102851-51-4 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



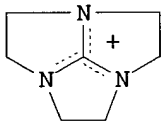
L30 ANSWER 81 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:207243 CAPLUS
DOCUMENT NUMBER: 104:207243
TITLE: I. Syntheses of selectively functionalized 9[ane]N3 and 12[ane]N3 cyclic triamines. II. Syntheses, complexation, and conformational studies of some azapodandocoronands
AUTHOR(S): Vachon, David John
CORPORATE SOURCE: Univ. New Hampshire, Durham, NH, USA
SOURCE: (1984) 321 pp. Avail.: Univ. Microfilms Int., Order No. DA8510484
From: Diss. Abstr. Int. B 1985, 46(3), 847
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable
IT 102202-73-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, complexation, and conformation of)
RN 102202-73-3 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris(2-methoxyethyl)- (9CI) (CA INDEX NAME)



L80 ANSWER 82 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1980:586289 CAPLUS
DOCUMENT NUMBER: 93:186289
TITLE: Transfer of hydrogen from orthoamides. Synthesis, structure, and reactions of hexahydro-6bH-2a,4a,6a-triazacyclopenta[cd]pentalene and perhydro-3a,6a,9a-triazaphenalene
AUTHOR(S): Erhardt, Jeanette M.; Grover, Edward R.; Wuest, James D.
CORPORATE SOURCE: Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA
SOURCE: Journal of the American Chemical Society (1980), 102(20), 6365-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 93:186289
GI

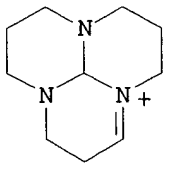


I, n=0
II, n=1

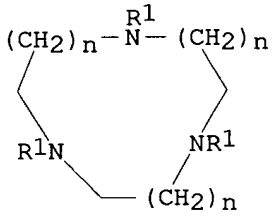


BF_4^-

III



IV



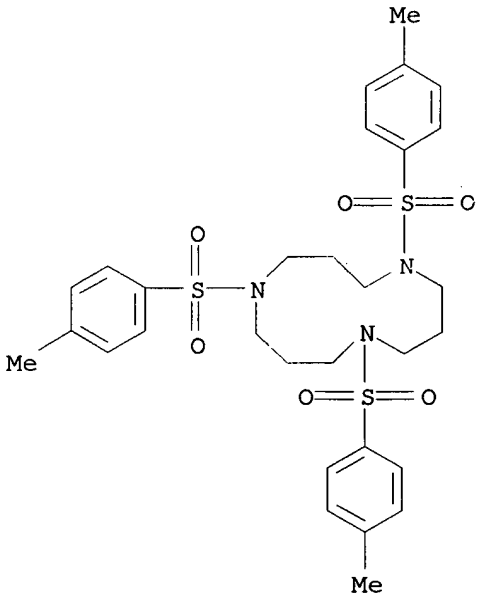
V

AB Hexahydro-6bH-2a,4a,6a-triazacyclopenta[c,d]pentalene (I) adopts a conformation in which the central C-H bond is syn-periplanar to three lone pairs; perhydro-3a,6a,9a-triazaphenalene (II) adopts a conformation in which the central C-H bond is anti-periplanar to three lone pairs. Orthoamide I readily reduces Ph3C+ BF4- to Ph3CH, and the product of oxidation is the guanidinium tetrafluoroborate III. Orthoamide II also reduces Ph3C+ BF4- to Ph3CH, but the central C-H bond is not broken: instead, steric or stereoelectronic factors appear to favor the formation of iminium ion IV. Both orthoamides efficiently reduce Me phenylglyoxylate in the presence of Mg(ClO4)2. I was prepared in 3 steps from triazonine V (R1 = tosyl, n = 1) and II in 7 steps from HN(CH2CH2CO2Et)2 via V (R1 = tosyl, n = 2).

IT 35980-67-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with hydrogen bromide)

RN 35980-67-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI)

(CA INDEX NAME)



L30 ANSWER 83 OF 83 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:140751 CAPLUS
DOCUMENT NUMBER: 76:140751
TITLE: Syntheses of some medium-sized cyclic triamines and their cobalt(III) complexes
AUTHOR(S): Koyama, Hiroyuki; Yoshino, Tamotsu
CORPORATE SOURCE: Fac. Sci., Kyushu Univ., Fukuoka, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1972), 45(2), 481-4
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Cyclic triamines (9-12-membered ring) form 3 mutually-adjacent 5-or 6-membered chelate rings on complexation, such as 1,4,7-triazacyclononane (I), 1,4,7-triazacyclodecane (II), 1,4,8-triazacycloundecane (III), and 1,5,9-triazacyclododecane (IV), which were isolated as their trihydrobromides. The complexation of I and II with a Co(III) salt gave metal complexes of a sandwich-type structure, such as [CoI2]Br3 and [CoII2]Br3.H2O. In the case of III, a complex [CoIIIBrCl2] was isolated. Formation of a Co(III) complex with IV in solution was inferred spectroscopically but no expected complex was isolated. The ligand-field strength increased in the following order: [Co(NH3)6]3+<[CoII2]3+<[Coen3]3+<[CoII2]3+.
IT 35980-67-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35980-67-7 CAPLUS
CN 1,5,9-Triazacyclododecane, 1,5,9-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)